

# Asymptotics of the mean-field Heisenberg model

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March 2, 2013

## Abstract

We consider the mean-field classical Heisenberg model and obtain detailed information about the magnetization by studying the model on a complete graph and sending the number of vertices to infinity. In particular, we obtain Cramèr- and Sanov-type large deviations principles for the magnetization and the empirical spin distribution and demonstrate a second-order phase transition in the Gibbs measures. We also study the asymptotics of the magnetization throughout the phase transition using Stein's method, proving central limit theorems in the sub- and supercritical phases and a nonnormal limit theorem at the critical temperature.

## 1 Introduction and summary of results

For many models of statistical mechanics, understanding their physical behavior starts with understanding the behavior of the corresponding mean-field model—which not only suggests how the physical model behaves, but also can predict rather precisely the physical behavior in high dimensions. There are two main statistical mechanical models of ferromagnetism: the simpler and better-understood Ising model, and the more realistic and more challenging (classical) Heisenberg model, on a lattice of dimension  $d$  with a spin  $\sigma_i \in \mathbb{S}^2$  at each lattice site  $i$ , the spin configuration  $\sigma \in (\mathbb{S}^2)^n$  having Hamiltonian energy in the absence of an external field (anisotropy):

$$H_n(\sigma) = - \sum_{i,j} J_{i,j} \langle \sigma_i, \sigma_j \rangle .$$

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\*Partially supported by NSF grants OISE-0730136 and DMS-1106770

†Partially supported by the American Institute of Mathematics and NSF grant DMS-0852898

The nearest-neighbor Heisenberg model has constant interaction  $J_{i,j} = J$  for nearest neighbors  $i$  and  $j$ , and no interaction  $J_{i,j} = 0$  otherwise. The mean-field version of the Heisenberg model has an averaged interaction  $J_{i,j} = \frac{1}{2n}$  for all  $i, j$  and can be understood as sending the dimension  $d \rightarrow \infty$  or considering the lattice to be a complete graph on  $n$  vertices and sending  $n \rightarrow \infty$ .

The related quantum Heisenberg model has nearest-neighbor interactions of spin matrices, and in dimensions three and higher, there is a celebrated proof of a phase transition to long-range order [7]. Such a result has been thus far intractable for the nearest-neighbor classical Heisenberg model, but the mean-field version is more amenable to rigorous analysis. In this article, we prove the existence of a second-order phase transition for the mean-field classical Heisenberg model, deriving a number of precise formulas and asymptotics for various physical quantities.

The simpler Ising model of ferromagnetism (the spins are in  $\{+1, -1\}$ ) is better understood, and our results parallel some recent developments for the mean-field version of the Ising model, called the Curie-Weiss model. It is believed that the Curie-Weiss model accurately describes the Ising model in dimensions greater than four, in the sense that they have the same critical exponents of various physical quantities (e.g., magnetization, free energy). The magnetization (the sum of the spins, appropriately normalized) in the Curie-Weiss model was shown by Ellis and Newman [10] to have a Gaussian law in the non-critical regimes and law that converges to the distribution with density proportional to  $e^{-x^4/12}$  at the critical temperature. Recently, it was shown by Chatterjee and Shao [3] that the magnetization at the critical temperature satisfies a Berry–Esseen type error bound of order  $1/\sqrt{n}$  for this non-central limit theorem. See also [2, 8] for analogous results on the Curie-Weiss-Potts model with an arbitrary finite number of discrete spins, and [1] for other related models.

There are a few results known for the Heisenberg model. In dimensions one and two, the classical Heisenberg model with nearest-neighbor interactions has no symmetry breaking, i.e., there is no phase transition to asymmetric macrostates above a critical temperature, e.g., [6]. By contrast, the classical Heisenberg model with long-range interactions or anisotropy (an external magnetic field) has a phase transition in two dimensions and higher, see [13] and references therein. And for classical, isotropic Heisenberg models with nearest-neighbor interactions in three dimensions and higher, the existence of a phase transition was shown using Fourier-based infrared bounds [11].

As for studying the mean-field classical Heisenberg model, the large-dimensional ( $d \rightarrow \infty$ ) limit of the nearest-neighbor model on  $\mathbb{Z}^d$ , with spins in  $\mathbb{S}^2$ , has the critical inverse temperature  $\beta_c = 3$ . Moreover, the large-dimensional limit is known to be a good approximation for high-dimensional models (as in Landau’s theory of second order phase transitions) in the sense that below the critical temperature, the magnetization is zero for all  $d$ , and above the critical temperature, the magnetization has the correct (non-zero) limit as  $d \rightarrow \infty$ .

The results in this article for the isotropic classical mean-field (in the complete graph sense) Heisenberg model include:

- Large deviation principles (LDPs) for the magnetization and the empirical spin distribution for each inverse temperature  $\beta \in [0, \infty)$  with explicit rate functions and relative entropies. (Section 2)

- Explicit formulas for the free energy and descriptions of the canonical macrostates and the corresponding second-order phase transition. (Section 2)
- An LDP for the empirical spin distribution with respect to the microcanonical ensemble, which has fixed energy, descriptions of the microcanonical macrostates and their second-order transition. (Section 2)
- A central limit theorem in the subcritical phase for the magnetization with the usual CLT scaling  $\sqrt{n}$ , using Stein's method. (Section 3)
- A CLT in the supercritical phase for the magnetization with a more complicated scaling, again using Stein's method. (Section 4)
- A nonnormal limit theorem for the magnetization at the critical temperature, with limiting density of the squared length proportional to  $t^5 e^{-3ct^2}$  (Section 5), using a new abstract Stein's method result for the nonnormal approximation (Appendix).

## 2 The model and large deviations results

We consider the isotropic mean-field classical Heisenberg model on a finite complete graph  $G_n$  with  $n$  vertices. That is, at each site of the graph is a spin living in  $\Omega = \mathbb{S}^2$ , so the state space is  $\Omega_n = (\mathbb{S}^2)^n$  with  $P_n$  the  $n$ -fold product of the uniform probability measure on  $\mathbb{S}^2$ . For this model, the mean-field Hamiltonian energy  $H_n : \Omega_n \rightarrow \mathbb{R}$  is:

$$H_n(\sigma) := -\frac{1}{2n} \sum_{i,j=1}^n \langle \sigma_i, \sigma_j \rangle.$$

The energy per particle is  $h_n(\sigma) = \frac{1}{n} H_n(\sigma)$ , and the canonical ensemble, or Gibbs measure, is the probability measure  $P_{n,\beta}$  on  $\Omega_n$  with density (with respect to  $P_n$ ):

$$f(\sigma) := \frac{1}{Z} \exp \left( \frac{\beta}{2n} \sum_{1 \leq i < j \leq n} \langle \sigma_i, \sigma_j \rangle \right) = \frac{1}{Z} e^{-\beta H_n(\sigma)} = \frac{1}{Z} e^{-n\beta h_n(\sigma)}.$$

Here the partition function is  $Z = Z_n(\beta) = \int_{\Omega_n} \exp \left( \frac{\beta}{2n} \sum_{i,j=1}^n \langle \sigma_i, \sigma_j \rangle \right) dP_n$ .

The empirical measure  $\mu_\sigma = \mu_{n,\sigma}$  of the spins  $\{\sigma_i\}$  is defined to be the random measure  $\mu_{n,\sigma} := \frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i}$  on  $\mathbb{S}^2$ . An interesting physical quantity is the empirical magnetization, defined by

$$S_n(\sigma) := n \int x d\mu_\sigma(x) = \sum_{i=1}^n \sigma_i.$$

A question of significant interest is the behavior of the magnetization as a function of the inverse temperature  $\beta$  in the Gibbs measures, so we begin by stating some large deviations principles for the  $\mu_{n,\sigma}$ . The first is an LDP (large deviations principle) for  $\mu_{n,\sigma}$  in the case that  $\beta = 0$ , which is an immediate consequence of Sanov's theorem (see; e.g. [5]).

**Proposition 1.** Let  $\{\sigma_i\}_{i=1}^n$  be i.i.d. uniform random variables on  $\mathbb{S}^2$  and let  $\mu_{n,\sigma} := \frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i}$ . For a probability measure  $\nu$  on  $\mathbb{S}^2$ , define the relative entropy of  $\nu$  with respect to the uniform probability measure  $\mu$  by

$$H(\nu \mid \mu) := \begin{cases} \int_{\mathbb{S}^2} f \log(f) d\mu & f := \frac{d\nu}{d\mu} \text{ exists;} \\ \infty & \text{otherwise.} \end{cases}$$

Let  $M_1(\mathbb{S}^2)$  denote the probability measures on  $\mathbb{S}^2$  with the weak-\* topology. Then for  $\Gamma$  a Borel subset of  $M_1(\mathbb{S}^2)$ ,

$$-\inf_{\nu \in \Gamma^\circ} H(\nu \mid \mu) \leq \liminf_{n \rightarrow \infty} \frac{1}{n} \log P_n[\mu_{n,\sigma} \in \Gamma] \leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log P_n[\mu_{n,\sigma} \in \Gamma] \leq -\inf_{\nu \in \overline{\Gamma}} H(\nu \mid \mu);$$

that is, the random measures  $\mu_{n,\sigma}$  satisfy an LDP with rate function  $H(\cdot \mid \mu)$ .

**Remark 2.** As a corollary of the Sanov-type LDP above, or independently, one can prove a Cramér-type LDP for the magnetization  $M_n := \frac{1}{n} \sum_{i=1}^n \sigma_i$  itself. Specifically, for the i.i.d. uniform random points  $\{\sigma_i\}_{i=1}^n$  on  $\mathbb{S}^2 \subseteq \mathbb{R}^3$ , the magnetization laws  $\mu_n := \mathcal{L}(M_n)$  satisfy an LDP with rate function  $I$ :

$$P_n(M_n \simeq x) \simeq e^{-nI(x)},$$

where  $I(x) = c|x| - \log\left(\frac{\sinh(c)}{c}\right) = c \coth(c) - 1 + \log\left(\frac{c}{\sinh(c)}\right)$ .

An LDP for the magnetization with respect to the Gibbs measures can also be proved, and we do this in the general case by deducing from Proposition 1 an LDP for the empirical spins  $\mu_{n,\sigma}$  with respect to the Gibbs measures for  $\beta > 0$ , making use of equivalence of ensembles (see [9]). The hidden (Polish) space is  $M_1(\mathbb{S}^2)$ , the set of Borel probability measures on  $\mathbb{S}^2$  equipped with the weak-\* topology. The hidden process is  $\{\mu_{n,\sigma}\}_{n=1}^\infty$  as in the theorem above, which satisfies an LDP with rate function  $H(\cdot \mid \mu)$ . The representation in question here is of the energy per particle, rather than the Hamiltonian itself:

$$h_n(\sigma) = -\frac{1}{2n^2} \sum_{i,j=1}^n \langle \sigma_i, \sigma_j \rangle = -\frac{1}{2} \left\langle \int_{\mathbb{S}^2} x d\mu_{n,\sigma}(x), \int_{\mathbb{S}^2} x d\mu_{n,\sigma}(x) \right\rangle = -\frac{1}{2} \left| \int_{\mathbb{S}^2} x d\mu_{n,\sigma}(x) \right|^2;$$

we define  $\tilde{h} : M_1(\mathbb{S}^2) \rightarrow \mathbb{R}$  by  $\tilde{h}(\nu) := -\frac{1}{2} \left| \int_{\mathbb{S}^2} x d\nu(x) \right|^2$ . Note that the expression inside the norm is simply the center of mass of the measure  $\nu$ .

We immediately obtain an LDP for the empirical measure of the spins at positive temperature by applying the equivalence of ensembles argument [9] to

$$z_n(\beta) := \int_{\Omega_n} e^{-\beta h_n} dP_n \quad \text{and} \quad p_{n,\beta}(B) := \frac{1}{z_n(\beta)} \int_B e^{-\beta h_n} dP_n.$$

**Proposition 3.** With notation as above, the  $\mu_{n,\sigma}$  satisfy an LDP with respect to the Gibbs measures  $P_{n,\beta} := p_{n,\beta}$  on  $M_1(\mathbb{S}^2)$  with rate function

$$I_\beta(\nu) := H(\nu \mid \mu) - \frac{\beta}{2} \left| \int_{\mathbb{S}^2} x d\nu(x) \right|^2 - \varphi(\beta), \tag{1}$$

where the free energy  $\varphi(\beta) := -\lim_{n \rightarrow \infty} \frac{1}{n} \log z_n(n\beta) = -\lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(\beta)$  exists and is given by

$$\varphi(\beta) = \inf_{\nu \in M_1(\mathbb{S}^2)} \left[ H(\nu \mid \mu) - \frac{\beta}{2} \left| \int_{\mathbb{S}^2} x d\nu(x) \right|^2 \right]. \quad (2)$$

Moreover:

- (a) The set of canonical macrostates  $\mathcal{E}_\beta := \{\nu : I_\beta(\nu) = 0\}$  is a non-empty, compact subset of  $M_1(\mathbb{S}^2)$ .
- (b) Non-macrostates are exponentially unlikely.
- (c) For every  $\beta > 0$ , every subsequence of  $P_{n,\beta}\{\mu_{n,\sigma} \in \cdot\}$  has a subsubsequence converging weakly to  $\Pi_\beta$ , a probability measure on  $M_1(\mathbb{S}^2)$  concentrated on  $\mathcal{E}_\beta$ , i.e.,  $\Pi_\beta(\mathcal{E}_\beta^c) = 0$ . In the case that  $\mathcal{E}_\beta = \{\nu\}$  for one  $\nu \in M_1(\mathbb{S}^2)$ , then the whole sequence converges weakly to  $\delta_\nu$ .

To identify the measures in  $\mathcal{E}_\beta$ , first observe that if  $f = \frac{d\nu}{d\mu}$  then  $H(\nu \mid \mu)$  depends only on the value distribution of  $f$ ; that is, (roughly speaking) once the values that  $f$  takes on the frequency with which they are taken on are fixed, the first term is determined. It is then easy to see that the expression  $|\int x d\nu(x)|$  is maximized (for a given value distribution) for corresponding densities which are symmetric about a fixed pole and decreasing as the distance from the pole increases. Consider, then, the case that  $f = \frac{d\nu}{d\mu}$ , a density that is symmetric about the north pole and decreasing away from the pole. That is,  $\nu_g$  is the measure with density  $f(x, y, z) = g(z)$  which is increasing in  $z$ . Then

$$\begin{aligned} H(\nu_g \mid \mu) &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi g(\cos(\theta)) \log[g(\cos(\theta))] \sin(\theta) d\theta d\varphi \\ &= \frac{1}{2} \int_{-1}^1 g(x) \log[g(x)] dx. \end{aligned}$$

By the same substitution,

$$\int_{\mathbb{S}^2} v d\nu_g(v) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \int_{-1}^1 \frac{xg(x)}{2} dx.$$

The problem is thus to minimize

$$\frac{1}{2} \int_{-1}^1 g(x) \log[g(x)] dx - \frac{\beta}{2} \left( \int_{-1}^1 \frac{xg(x)}{2} dx \right)^2$$

for  $g : [-1, 1] \rightarrow \mathbb{R}_+$  such that  $\frac{1}{2} \int_{-1}^1 g(x) dx = 1$  and  $g$  is increasing. Observe that

$$\frac{1}{2} \int_{-1}^1 g(x) \log[g(x)] dx = \frac{1}{2} \int_{-1}^1 g(x) \log \left[ \frac{g(x)}{2} \right] dx + \log(2) = -h \left( \frac{g}{2} \right) + \log(2),$$

where  $h(\varphi)$  is the (usual) entropy of the density  $\varphi$ .

Now fix the value of  $|\int x d\nu(x)| \in [0, 1]$  and minimize  $\frac{1}{2} \int_{-1}^1 g(x) \log[g(x)] dx$  over the  $\nu \in M_1(\mathbb{S}^2)$  corresponding to this value; this is a constrained entropy maximization problem, for which known results [4] imply:

**Proposition 4.** Consider the class of  $f : [-1, 1] \rightarrow \mathbb{R}_+$  such that

- $\int_{-1}^1 f(x)dx = 1$ , and
- $\left| \int_{-1}^1 x f(x)dx \right| = c$ .

Then  $f^*(x) = k_1 e^{k_2 x}$  uniquely maximizes  $h(f)$  over the densities satisfying these conditions.

Now, to determine  $k_1, k_2$  (their formulas are in the next proposition), observe that for  $f^*$  to satisfy the first condition,

$$1 = \int_{-1}^1 k_1 e^{k_2 x} dx = \frac{2k_1 \sinh(k_2)}{k_2},$$

and thus

$$k_1 = \frac{k_2}{2 \sinh(k_2)}.$$

For the second condition,

$$c = k_1 \int_{-1}^1 x e^{k_2 x} dx = k_1 \left[ \frac{2 \cosh(k_2)}{k_2} - \frac{2 \sinh(k_2)}{k_2^2} \right] = \coth(k_2) - \frac{1}{k_2}.$$

Take  $g^* = 2f^*$ ; considering all  $c \in [0, 1]$  and requiring  $g^*$  to be increasing corresponds to considering all  $k_2 \in [0, \infty)$ . In that case, we need to minimize

$$\begin{aligned} & \frac{1}{2} \int_{-1}^1 g^*(x) \log[g^*(x)] dx - \frac{\beta}{2} c^2 \\ &= \log \left( \frac{k_2}{\sinh(k_2)} \right) + k_2 \coth(k_2) - 1 - \frac{\beta}{2} \left( \coth(k_2) - \frac{1}{k_2} \right)^2 =: \Phi_\beta(k_2) \end{aligned} \quad (3)$$

over all  $k_2 \in [0, \infty)$ .

This optimization problem leads to a critical value of the inverse temperature  $\beta_c = 3$ , and the phase transition is a continuous one (2nd order in physics parlance). Below the transition, the only macrocanonical state is the uniform distribution, and then increasing  $\beta$  across the critical threshold, a spherically symmetric family of distributions with a preferred direction appears. At first the direction is hardly preferred at all, but with increasing  $\beta$  the preferred direction becomes more strongly preferred, so that in the zero temperature limit  $\beta \rightarrow \infty$ , the macrostates are point masses.

More precisely, the following results are proved in the appendix and summarized here:

**Proposition 5.** The free energy  $\varphi$  as characterized in Theorem 3 has the formula (lemma 15):

$$\varphi(\beta) = \begin{cases} 0, & \text{if } \beta < 3, \\ \Phi_\beta(g^{-1}(\beta)), & \text{if } \beta \geq 3, \end{cases}$$

where  $\Phi_\beta$  is defined above in (3) and

$$g(x) := \frac{x}{\coth x - 1/x} = \beta.$$

**Second-order phase transition:** The function  $\varphi$  and its derivative  $\varphi'$  are continuous at the critical threshold  $\beta = 3$ , so the phase transition is continuous.

(a) In the subcritical case,  $\beta \leq 3$ , the expression (3) is minimized for  $k_2 = 0$ , and the corresponding  $k_1 = 0$ , so that the minimizing function  $f^* = 1$  and hence the canonical macrostates in the subcritical case are uniform:  $\mathcal{E}_\beta = \{\mu\}$ .

(b) In the supercritical case,  $\beta > 3$ , the minimizing  $k_2$  has limit  $\lim_{\beta \downarrow \beta_c} k_2 = 0$ .

The macro states  $\mathcal{E}_\beta = \{\nu_x\}_{x \in \mathbb{S}^2}$ , where  $\nu_x$  is the rotation of the measure  $\nu$  considered above, such that  $x$  plays the role of the north pole.

One can furthermore use the computations above (or work directly) to derive an explicit formula for the rate function for the LDP of the magnetization  $\frac{1}{n} \sum_{i=1}^n \sigma_i$ . Specifically, one has the following.

**Theorem 6.** Let  $\{\sigma\}_{i=1}^n$  be a configuration of spins distributed according to the Gibbs measure described above, and let  $S_n := \sum_{i=1}^n \sigma_i$ . Then for a Borel set  $\Gamma \in \mathbb{R}$ ,

$$-\inf_{x \in \Gamma^\circ} I_\beta(x) \leq \liminf_{n \rightarrow \infty} \frac{1}{n} \log P_{n,\beta} \left[ \frac{|\beta S_n|}{n} \in \Gamma \right] \leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log P_{n,\beta} \left[ \frac{|\beta S_n|}{n} \in \Gamma \right] \leq -\inf_{x \in \bar{\Gamma}} I_\beta(x)$$

where

$$I_\beta(x) = c \coth(c) - 1 - \log \left( \frac{\sinh(c)}{c} \right) - \frac{\beta}{2} \left| \coth(c) - \frac{1}{c} \right|^2,$$

and  $c$  is the unique element of  $\mathbb{R}^+$  such that  $|x| = \coth(c) - \frac{1}{c}$ .

Also of interest is the microcanonical ensemble, in which one fixes the energy per particle, and the following result gives an LDP in that case using the results of [9].

**Proposition 7.** Since the empirical measure of the spins  $\mu_{n,\sigma} = \frac{1}{n} \sum \delta_{\sigma_i}$  satisfies an LDP with respect to the product measure  $P_n$  with rate  $H(\cdot | \mu)$ , we have the following:

(a) The energies  $\tilde{h}(\mu_{n,\sigma})$  and  $H_n$  satisfy LDPs with respect to  $P_n$  with rate  $J$ , called the microcanonical entropy, defined for a fixed value  $u$  of the energy by:

$$J(u) := \inf \{ H(\nu | \mu) : \nu \in M_1(\mathbb{S}^2), \tilde{h}(\nu) = u \}.$$

The free energy  $\varphi$  is a Legendre-Fenchel transform:  $\varphi(\beta) = \inf_{u \in \mathbb{R}} \{ \beta u + J(u) \}$ .

(b) If  $u \in \text{dom}(J)$ , then  $\mu_{n,\sigma}$  satisfies an LDP with respect to the microcanonical Gibbs measure

$$P_n^{u,r}(A) := \frac{1}{Z_u} \int_A \mathbb{K}_{\{H_n \in [u+r, u-r]\}} dP_n,$$

where  $Z_u := \int_{\mathbb{S}^2} \mathbb{K}_{\{H_n \in [u+r, u-r]\}} dP_n$ , and with microcanonical rate function

$$I^u(\nu) := \begin{cases} H(\nu | \mu) - J(u), & \text{if } -\frac{1}{2} \langle \nu, \nu \rangle = u; \\ \infty, & \text{otherwise.} \end{cases}$$

That is,

$$-\inf_{\nu \in \Gamma^\circ} I^u(\nu) \leq \lim_{r \rightarrow 0} \liminf_{n \rightarrow \infty} \frac{1}{n} \log P_n^{u,r}(\Gamma) \leq \lim_{r \rightarrow 0} \limsup_{n \rightarrow \infty} \frac{1}{n} \log P_n^{u,r}(\Gamma) \leq -\inf_{\nu \in \bar{\Gamma}} I^u(\nu);$$

(c) *The microcanonical macrostates are*

$$\mathcal{E}^u := \{\nu : H(\nu \mid \mu) = J(u), \tilde{h}(\nu) = u\}.$$

Again, it suffices to restrict our attention to symmetric densities  $\frac{d\nu}{d\mu}$ , symmetric about a pole with unit vector  $\hat{z}$ , i.e.,  $\int v d\nu(v) = c\hat{z}$ , because symmetrizing about the  $z$ -axis reduces relative entropy: Recall that  $d\mu = d\mu_z \frac{dz}{2}$ , where  $\mu_z$  is the uniform measure on the circle of radius  $\sqrt{1-z^2}$ . Let  $\tilde{f}(z) := \int f(x, y, z) d\mu_z(x, y)$ , which is the symmetrized version of  $f$  about the  $z$ -axis. Now, the function  $g(x) = x \log(x)$  is convex, so by Jensen's inequality,

$$\begin{aligned} \tilde{f}(z) \log[\tilde{f}(z)] &= g\left(\int f(x, y, z) d\mu_z(x, y)\right) \leq \int g(f(x, y, z)) d\mu_z(x, y) \\ &= \int f(x, y, z) \log[f(x, y, z)] d\mu_z(x, y). \end{aligned}$$

Integrating both sides with respect to  $\frac{dz}{2}$  shows that  $H(\tilde{\nu} \mid \mu) \leq H(\nu \mid \mu)$ , where  $\nu$  and  $\tilde{\nu}$  are respectively the measures with densities  $f$  and  $\tilde{f}$ .

We can compute  $J$  to be

$$J(u) = \inf \left\{ H(\tilde{\nu} \mid \mu) : \left( \frac{1}{2} \int_{-1}^1 x \tilde{f}(x) dx \right)^2 = -2u, \frac{1}{2} \int \tilde{f}(x) dx = 1 \right\},$$

and then simplify it using the previous result on maximizing entropy, with  $k_2$  solving  $\coth k_2 - \frac{1}{k_2} = \sqrt{-2u}$ :

$$J(u) = \log \left( \frac{k_2}{\sinh k_2} \right) + k_2 \sqrt{-2u}.$$

The microcanonical entropy is

$$I^u(\tilde{\nu}) = -h(\tilde{f}/2) + \log 2 - J(u), \text{ if } \left( \frac{1}{2} \int_{-1}^1 x \tilde{f}(x) dx \right)^2 = -2u.$$

The domain of  $J$  is  $(-\frac{1}{2}, 0]$ , and the microcanonical macrostates  $\mathcal{E}^u$  consist of rotations to any direction of  $\tilde{\nu}$  with density

$$\tilde{f} = \frac{k_2}{\sinh k_2} e^{k_2 x}, \text{ where } \coth k_2 - \frac{1}{k_2} = \sqrt{-2u}.$$

In particular,  $\mathcal{E}^0 = \{\mu\}$ , the completely disordered phase, and for energies close to zero  $-\frac{1}{2} \ll u < 0$ , there is the expansion  $J(u) \simeq -3u - \frac{9}{2}u^2 + \dots$ , and  $k_2 \simeq 3\sqrt{-2u}$ . Thus the microcanonical macrostates for small energy are  $\mathcal{E}^u = \{\nu_x\}_{x \in \mathbb{S}^2}$ , where  $\nu_x$  is the rotation of  $\tilde{\nu}$  to the  $x$  direction, again a continuous transition to the ordered phase.



### 3 The magnetization in the subcritical phase

We restrict our attention to the subcritical (disordered) regime  $\beta < 3$  in this section.

First note that each of the spins  $\sigma_i$  has a uniform marginal distribution, because the density of the Gibbs measure is rotationally invariant. In particular,  $\mathbb{E}[\sigma_i] = 0$  for each  $i$ , and thus the expected magnetization is zero.

To compute the variance of the total magnetization  $S_n := \sum_{i=1}^n \sigma_i$ , note that  $\mathbb{E} \langle \sigma_i, \sigma_i \rangle = 1$  for each  $i$ ; moreover, by the symmetry of the Gibbs measure,  $\mathbb{E} \langle \sigma_i, \sigma_j \rangle$  is the same for every pair  $i \neq j$ . Now, conditional on  $\{\sigma_j\}_{j \neq 1}$ , the density of  $\sigma_1$  with respect to uniform measure on  $\mathbb{S}^2$  is given by

$$\frac{1}{Z_1} \exp \left[ \frac{\beta}{n} \sum_{j \neq 1} \langle \theta, \sigma_j \rangle \right],$$

where the normalization is  $Z_1 = \int_{\mathbb{S}^2} \exp \left[ \frac{\beta}{n} \sum_{j \neq 1} \langle \theta, \sigma_j \rangle \right] d\mu(\theta)$ . For fixed  $i \in \{1, \dots, n\}$ , let  $\sigma^{(i)} := \sum_{j \neq i} \sigma_j$ . Note that  $d\mu(\theta) = \frac{\sin \alpha}{4\pi} d\alpha d\phi$ , where  $(\alpha, \phi)$  are spherical coordinates;  $Z_1$  is therefore given by

$$Z_1 = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi e^{c \cos(\alpha)} \sin(\alpha) d\alpha d\phi = \frac{\sinh(c)}{c},$$

where  $c = \frac{\beta |\sigma^{(1)}|}{n}$ . Now, from the conditional density above,

$$\begin{aligned} \mathbb{E} [\sigma_1 | \{\sigma_j\}_{j \neq 1}] &= \frac{1}{Z_1} \int_{\mathbb{S}^2} \theta \exp \left[ \frac{\beta}{n} \sum_{j \neq 1} \langle \theta, \sigma_j \rangle \right] d\mu(\theta) \\ &= \frac{1}{Z_1} \int_{\mathbb{S}^2} \left\langle \theta, \frac{\sigma^{(1)}}{|\sigma^{(1)}|} \right\rangle \left( \frac{\sigma^{(1)}}{|\sigma^{(1)}|} \right) \exp \left[ \frac{\beta}{n} \langle \theta, \sigma^{(1)} \rangle \right] d\mu(\theta) \\ &= \left[ \frac{1}{4\pi Z_1} \int_0^{2\pi} \int_0^\pi \cos(\alpha) \sin(\alpha) e^{\frac{\beta |\sigma^{(1)}| \cos(\alpha)}{n}} d\alpha d\phi \right] \left( \frac{\sigma^{(1)}}{|\sigma^{(1)}|} \right) \\ &= \left[ \coth \left( \frac{\beta |\sigma^{(1)}|}{n} \right) - \frac{n}{\beta |\sigma^{(1)}|} \right] \left( \frac{\sigma^{(1)}}{|\sigma^{(1)}|} \right). \end{aligned}$$

Recall that if  $\beta < 3$ , then  $\frac{\beta |\sigma^{(1)}|}{n} = o(1)$  with probability exponentially close to one. Expanding about zero gives that for  $x$  small,  $\coth(x) - \frac{1}{x} \approx \frac{x}{3}$ , and so we have that if  $\beta < 3$ , then

$$\mathbb{E} [\sigma_1 | \{\sigma_j\}_{j \neq 1}] \approx \frac{\beta \sigma^{(1)}}{3n} = \frac{\beta}{3n} \sum_{i \neq 1} \sigma_i,$$

(this argument will be made precise below). It follows by taking inner product of both sides with  $\sigma_2$  followed by expectation that

$$\mathbb{E} \langle \sigma_1, \sigma_2 \rangle \approx \frac{\beta}{3n} \mathbb{E} \left\langle \sum_{j \neq 1} \sigma_j, \sigma_2 \right\rangle = \frac{\beta}{3n} [1 + (n-2) \mathbb{E} \langle \sigma_1, \sigma_2 \rangle],$$

and thus

$$\mathbb{E} \langle \sigma_1, \sigma_2 \rangle \approx \frac{\beta}{3n - \beta(n-2)} \approx \frac{\beta}{n(3-\beta)}.$$

Finally,

$$\mathbb{E}|S_n|^2 = n\mathbb{E}|\sigma_1|^2 + n(n-1)\mathbb{E} \langle \sigma_1, \sigma_2 \rangle \approx \frac{3n}{3-\beta}.$$

We therefore consider the scaled magnetization  $M = \sqrt{\frac{3-\beta}{n}} \sum_{i=1}^n \sigma_i$ ; the remainder of the section is devoted to proving the following central limit theorem for  $M$ .

**Theorem 8.** *For  $\beta < 3$ , there is a constant  $c_\beta$  depending only on  $\beta$  such that for  $M = \sqrt{\frac{3-\beta}{n}} \sum_{i=1}^n \sigma_i$ ,*

$$\sup_{g: M_1(g), M_2(g) \leq 1} |\mathbb{E}g(M) - \mathbb{E}g(Z)| \leq \frac{c_\beta \log(n)}{\sqrt{n}}$$

where  $M_1(g)$  is the Lipschitz constant of  $g$ ,  $M_2(g)$  is the maximum operator norm of the Hessian of  $g$ , and  $Z$  is a standard Gaussian random vector in  $\mathbb{R}^3$ .

The theorem is proved as an application of the following abstract normal approximation theorem from [14].

**Theorem 9.** *Let  $(X, X')$  be an exchangeable pair of random vectors in  $\mathbb{R}^d$ . Let  $\mathcal{F}$  be a  $\sigma$ -algebra with  $\sigma(X) \subseteq \mathcal{F}$ , and suppose that there is an invertible matrix  $\Lambda$ , a symmetric, positive definite matrix  $\Sigma$ , an  $\mathcal{F}$ -measurable random vector  $E$  and an  $\mathcal{F}$ -measurable random matrix  $E'$  such that*

(a)

$$\mathbb{E}[X' - X | \mathcal{F}] = -\Lambda X + E$$

(b)

$$\mathbb{E}[(X' - X)(X' - X)^T | \mathcal{F}] = 2\Lambda\Sigma + E'.$$

Then for  $g \in C^2(\mathbb{R}^d)$ ,

$$\begin{aligned} |\mathbb{E}g(X) - \mathbb{E}g(\Sigma^{1/2}Z)| &\leq M_1(g)\|\Lambda^{-1}\|_{op} \left[ \mathbb{E}|E| + \frac{1}{2}\|\Sigma^{-1/2}\|_{op}\mathbb{E}\|E'\|_{H.S.} \right] \\ &\quad + \frac{\sqrt{2\pi}}{24}M_2(g)\|\Sigma^{-1/2}\|_{op}\|\Lambda^{-1}\|_{op}\mathbb{E}|X' - X|^3, \end{aligned} \tag{4}$$

where  $M_1(g)$  is the Lipschitz constant of  $g$  and  $M_2(g)$  is the maximum operator norm of  $\text{Hess}(g)$ .

The first step in applying the theorem is to construct an exchangeable pair  $(M, M')$ . As is frequently the case, the exchangeable pair will first be constructed on the level of configurations, and then descend to the magnetization. Given a fixed configuration  $\sigma$ , construct a new configuration  $\sigma'$  by letting  $I$  be distributed uniformly in  $\{1, \dots, n\}$  and replacing  $\sigma_I$  by  $\sigma'_I$ , distributed according to the conditional distribution of the  $I$ -th spin,

given  $\{\sigma_j : j \neq I\}$ , and defining  $\sigma'_j := \sigma_j$  for  $j \neq I$ . Then  $M = \sqrt{\frac{3-\beta}{n}} \sum_{i=1}^n \sigma_i$  and  $M' = M(\sigma') = M - \sqrt{\frac{3-\beta}{n}} \sigma_I + \sqrt{\frac{3-\beta}{n}} \sigma'_I$ ; that is,  $M$  is the magnetization of the configuration in which a random spin has been replaced via the Gibbs sampler. For notational convenience, let  $a := \sqrt{3-\beta}$ . Then, using the computation above,

$$\begin{aligned} \mathbb{E} [M' - M | \sigma] &= -\frac{a}{n^{3/2}} \sum_{i=1}^n [\sigma_i - \mathbb{E} [\sigma_i | \{\sigma_j\}_{j \neq i}]] \\ &= -\frac{1}{n} M + \frac{a}{n^{3/2}} \sum_{i=1}^n \left[ \coth \left( \frac{\beta |\sigma^{(i)}|}{n} \right) - \frac{n}{\beta |\sigma^{(i)}|} \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right). \end{aligned}$$

Now, since  $\beta < 3$ , it is known that  $\frac{\beta |\sigma^{(i)}|}{n} = o(1)$  with probability exponentially close to 1. We therefore use the expansion of  $\coth(x) - \frac{1}{x}$  near zero to write

$$\begin{aligned} \mathbb{E} [M' - M | \sigma] &= -\frac{1}{n} M + \left( \frac{a}{3n^{5/2}} \sum_{i=1}^n \sum_{j \neq i} \beta \sigma_j \right) \\ &\quad + \frac{a}{n^{3/2}} \sum_{i=1}^n \left[ \coth \left( \frac{\beta |\sigma^{(i)}|}{n} \right) - \frac{n}{\beta |\sigma^{(i)}|} - \frac{\beta |\sigma^{(i)}|}{3n} \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right). \end{aligned}$$

Note that

$$\frac{a}{3n^{5/2}} \sum_{i=1}^n \sum_{j \neq i} \beta \sigma_j = \frac{1}{3n^2} \sum_{i=1}^n \left( \beta M - \frac{a \beta \sigma_i}{\sqrt{n}} \right) = \frac{1}{n} \left( \frac{\beta}{3} - \frac{\beta}{3n} \right) M.$$

The matrix  $\Lambda$  of Theorem 9 is thus  $\frac{1-\beta}{n} Id$  and

$$E = -\frac{\beta}{3n^2} M + \frac{a}{n^{3/2}} \sum_{i=1}^n \left[ \coth \left( \frac{\beta |\sigma^{(i)}|}{n} \right) - \frac{n}{\beta |\sigma^{(i)}|} - \frac{\beta |\sigma^{(i)}|}{3n} \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right).$$

We next compute  $\mathbb{E} [(M' - M)(M' - M)^T | \sigma]$ . By the same considerations as above, this is given by

$$\begin{aligned} \mathbb{E} [(M' - M)(M' - M)^T | \sigma] &= \frac{a^2}{n^2} \sum_{i=1}^n \frac{1}{Z_i} \int_{\mathbb{S}^2} (\theta - \sigma_i)(\theta - \sigma_i)^T \exp \left[ \frac{\beta}{n} \sum_{j \neq i} \langle \sigma_j, \theta \rangle \right] d\mu(\theta) \\ &= \frac{a^2}{n^2} \sum_{i=1}^n \frac{1}{Z_i} \int_{\mathbb{S}^2} [\theta \theta^T - \sigma_i \theta^T - \theta \sigma_i^T + \sigma_i \sigma_i^T] \exp \left[ \frac{\beta}{n} \sum_{j \neq i} \langle \sigma_j, \theta \rangle \right] d\mu(\theta). \end{aligned}$$

Letting  $\theta = \theta_1 + \theta_2$ , where  $\theta_1$  is the projection of  $\theta$  onto the direction of  $\sigma^{(i)}$  and  $\theta_2$  is the orthogonal complement, the first term of the last expression is given by

$$\frac{1}{Z_i} \int_{\mathbb{S}^2} [\theta_1 \theta_1^T + \theta_2 \theta_2^T] \exp \left[ \frac{\beta}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta), \quad (5)$$

since the cross terms vanish by symmetry. To compute it, write  $r_i = \frac{\sigma^{(i)}}{|\sigma^{(i)}|}$ , so that  $\theta_1 = \langle \theta, r_i \rangle r_i$ , and  $\theta_1 \theta_1^T = |\langle \theta, r_i \rangle|^2 r_i r_i^T$ ; setting  $c := \frac{\beta |\sigma^{(i)}|}{n}$ ,

$$\frac{1}{Z_i} \int_{\mathbb{S}^2} \theta_1 \theta_1^T \exp \left[ \frac{\beta}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta) = \frac{1}{Z_i} \left( \int_{\mathbb{S}^2} |\langle \theta, r_i \rangle|^2 \exp [c \langle r_i, \theta \rangle] d\mu(\theta) \right) r_i r_i^T.$$

(Recall that  $r_i r_i^T$  is orthogonal projection onto the span of  $r_i$  in  $\mathbb{R}^3$ .) In spherical coordinates (with  $r_i$  playing the role of the north pole), the integral is then given by

$$\frac{1}{4\pi Z_i} \int_0^{2\pi} \int_0^\pi |\cos \alpha|^2 \exp [c \cos \alpha] \sin \alpha d\alpha d\phi.$$

Evaluating and using the established formula for  $Z_i$  yields

$$\frac{1}{Z_i} \int_{\mathbb{S}^2} \theta_1 \theta_1^T \exp \left[ \frac{1}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta) = \frac{c^2 - 2c \coth(c) + 2}{c^2} P_i,$$

where  $P_i$  is orthogonal projection onto  $r_i$ .

Now, for the second half of (5), let  $(\theta_x, \theta_y)$  be a representation of  $\theta_2$  in orthonormal coordinates within  $r_1^\perp$ . Note that

$$\int_{\mathbb{S}^2} \theta_x \theta_y e^{c \langle r_i, \theta \rangle} d\mu(\theta) = 0$$

by symmetry. Expanding in polar coordinates,

$$\begin{aligned} \int_{\mathbb{S}^2} \theta_y^2 e^{c \langle r_i, \theta \rangle} d\mu(\theta) &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi \sin(\alpha)^3 \cos(\phi)^2 e^{c \cos(\alpha)} d\alpha d\phi \\ &= \frac{1}{4} \int_0^\pi \sin(\alpha)^3 e^{c \cos(\alpha)} d\alpha \\ &= \frac{c \cosh(c) - \sinh(c)}{c^3}. \end{aligned}$$

Of course, the value is the same when  $\theta_y^2$  is replaced by  $\theta_x^2$ , and thus

$$\begin{aligned} \frac{1}{Z_i} \int_{\mathbb{S}^2} \theta_2 \theta_2^T \exp \left[ \frac{\beta}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta) &= \frac{c \cosh(c) - \sinh(c)}{Z_i c^3} P_i^\perp \\ &= \left[ \frac{\coth(c)}{c} - \frac{1}{c^2} \right] P_i^\perp, \end{aligned}$$

where  $P_i^\perp$  is the orthogonal projection onto  $r_i^\perp$ .

Formulae for the middle terms follow from the computations above:

$$\frac{1}{Z_i} \int_{\mathbb{S}^2} \theta \sigma_i^T \exp \left[ \frac{\beta}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta) = \left[ \coth(c) - \frac{1}{c} \right] r_i \sigma_i^T.$$

The next term is just the transpose of this one.

Finally, the last term is trivial:

$$\frac{1}{Z_i} \int_{\mathbb{S}^2} \sigma_i \sigma_i^T \exp \left[ \frac{\beta}{n} \langle \sigma^{(i)}, \theta \rangle \right] d\mu(\theta) = \sigma_i \sigma_i^T.$$

Collecting terms,

$$\begin{aligned} \mathbb{E} [(M' - M)(M' - M)^T | \sigma] &= \frac{a^2}{n^2} \sum_{i=1}^n \left\{ \left[ 1 - \frac{2c \coth(c) - 2}{c^2} \right] P_i + \left[ \frac{\coth(c)}{c} - \frac{1}{c^2} \right] P_i^\perp \right. \\ &\quad \left. - \left[ \coth(c) - \frac{1}{c} \right] (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T \right\}, \end{aligned}$$

where  $c = \frac{\beta |\sigma^{(i)}|}{n}$ . Recall that if  $c = o(1)$  then  $\coth(c) - \frac{1}{c} \approx \frac{c}{3}$ . In this case,

$$\begin{aligned} \mathbb{E} [(M' - M)(M' - M)^T | \sigma] &= \frac{a^2}{n^2} \sum_{i=1}^n \left\{ \frac{1}{3} P_i + \frac{1}{3} P_i^\perp - \frac{c}{3} (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T \right\} + E'' \\ &= \frac{a^2}{3n} Id + \frac{a^2}{n^2} \sum_{i=1}^n \sigma_i \sigma_i^T - \frac{a^2 c}{3n^2} \sum_{i=1}^n (r_i \sigma_i^T + \sigma_i r_i^T) + E'', \end{aligned} \tag{6}$$

where the error term  $E''$  incurred in this approximation is

$$\begin{aligned} E'' &= \frac{a^2}{n^2} \sum_{i=1}^n \left\{ \left[ \frac{2}{3} - \frac{2c \coth(c) - 2}{c^2} \right] P_i + \left[ \frac{\coth(c)}{c} - \frac{1}{c^2} - \frac{1}{3} \right] P_i^\perp \right. \\ &\quad \left. - \left[ \coth(c) - \frac{1}{c} - \frac{c}{3} \right] (r_i \sigma_i^T + \sigma_i r_i^T) \right\}. \end{aligned}$$

Observe further that, for the second-last term of (6), using  $r_i = \frac{\sigma^{(i)}}{|\sigma^{(i)}|}$  and  $c = \frac{\beta |\sigma^{(i)}|}{n}$  yields

$$\frac{a^2 c}{3n^2} \sum_{i=1}^n (r_i \sigma_i^T + \sigma_i r_i^T) = \frac{a^2 \beta}{3n^3} \sum_{i=1}^n \sum_{j \neq i} (\sigma_j \sigma_i^T + \sigma_i \sigma_j^T) = \frac{2\beta}{3n^2} M M^T - \frac{2a^2 \beta}{3n^3} \sum_{i=1}^n \sigma_i \sigma_i^T.$$

Putting the pieces together,

$$\begin{aligned} \mathbb{E} [(M' - M)(M' - M)^T | \sigma] &= \frac{a^2}{3n} \left[ Id + \frac{1}{n} \sum_{i=1}^n 3\sigma_i \sigma_i^T \right] - \frac{2\beta}{3n^2} M M^T + \frac{2\beta}{3n^4} \sum_{i=1}^n \sigma_i \sigma_i^T + E'' \\ &= \left( \frac{3 - \beta}{3n} \right) \left[ Id + \frac{1}{n} \sum_{i=1}^n 3\sigma_i \sigma_i^T \right] - \frac{2\beta}{3n^2} M M^T + \frac{2\beta}{3n^4} \sum_{i=1}^n \sigma_i \sigma_i^T + E''. \end{aligned}$$

Note that if  $X$  is uniformly distributed on the sphere, then if  $U \in \mathcal{O}_3$ ,

$$\mathbb{E}[X X^T] = \mathbb{E}[U X U^T U X^T U^T] = U \mathbb{E}[X X^T] U^T,$$

and thus  $\mathbb{E}[XX^T]$  is a scalar matrix. Moreover,  $\text{Tr}(XX^T) = 1$  since  $XX^T$  is a rank-one projection, and thus  $\mathbb{E}[\text{Tr}(XX^T)] = 1$  and so since  $\mathbb{E}[XX^T]$  is scalar, it follows that  $\mathbb{E}[XX^T] = \frac{1}{3}Id$ . That is,  $\mathbb{E}[\sigma_i \sigma_i^T] = \frac{1}{3}Id$  for each  $i$ . We therefore write

$$\mathbb{E}[(M' - M)(M' - M)^T | \sigma] = 2 \left( \frac{1 - \frac{\beta}{3}}{n} \right) \Sigma + E',$$

as in Theorem 9, with  $\Sigma = Id$  and

$$E' = \left( \frac{1 - \frac{\beta}{3}}{n} \right) \left[ \frac{1}{n} \sum_{i=1}^n 3\sigma_i \sigma_i^T - Id \right] - \frac{2\beta}{3n^2} MM^T + \frac{2\beta}{3n^4} \sum_{i=1}^n \sigma_i \sigma_i^T + E''.$$

Note in particular that the expected value of the first term of  $E'$  is zero.

To apply Theorem 9, various quantities need to be computed or estimated. Recall that  $\Lambda = \frac{1 - \frac{\beta}{3}}{n} Id$ , and thus  $\|\Lambda^{-1}\|_{op} = \frac{n}{1 - \frac{\beta}{3}}$ . Now, the first term of  $E$  is  $-\frac{\beta}{3n^2} M$ . Note that, while it was previously argued heuristically that  $\mathbb{E}|M|^2 \approx 3$ , one can in fact use the same argument together with the fact that  $\coth(x) - \frac{1}{x} \leq \frac{x}{3}$  (shown in the proof of Lemma 14) to show that  $\mathbb{E}|M|^2 \leq 3$ . It then follows that

$$\frac{\beta}{3n^2} \mathbb{E}|M| \leq \frac{\beta}{3n^2} \sqrt{\mathbb{E}|M|^2} \leq \frac{\beta}{\sqrt{3}n^2}.$$

To estimate the second half of  $E$ , fix  $\epsilon = \epsilon(n) \in (0, 1)$  to be chosen later. For notational convenience, let  $R(t) := \coth(t) - \frac{1}{t} - \frac{t}{3}$ ; observe that if  $t \leq \epsilon$  then  $|R(t)| < b\epsilon^2$ , where  $b$  is a universal constant. Then the second half of  $E$  can be estimated as

$$\begin{aligned} \frac{a}{n^{3/2}} \left| \sum_{i=1}^n \left[ R\left(\frac{\beta|\sigma^{(i)}|}{n}\right) \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right) \right| &\leq \frac{a}{n^{3/2}} \left| \sum_{i=1}^n \left[ R\left(\frac{\beta|\sigma^{(i)}|}{n}\right) \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right) \mathbb{1}_{\left(\frac{\beta|\sigma^{(i)}|}{n} \leq \epsilon\right)} \right| \\ &\quad + \frac{a}{n^{3/2}} \left| \sum_{i=1}^n \left[ R\left(\frac{\beta|\sigma^{(i)}|}{n}\right) \right] \left( \frac{\sigma^{(i)}}{|\sigma^{(i)}|} \right) \mathbb{1}_{\left(\frac{\beta|\sigma^{(i)}|}{n} > \epsilon\right)} \right| \\ &\leq \frac{ba\epsilon^2}{\sqrt{n}} + \frac{a}{n^{3/2}} \sum_{i=1}^n \mathbb{1}_{\left(\frac{\beta|\sigma^{(i)}|}{n} > \epsilon\right)}, \end{aligned}$$

making use of the fact that  $|R(\frac{\beta|\sigma^{(i)}|}{n})| \leq 1$  for any configuration  $\sigma$ . From the LDP for  $\sigma^{(i)}$ ,

$$\mathbb{P} \left[ \frac{\beta|\sigma^{(i)}|}{n} > \epsilon \right] \leq C \exp \left[ -\frac{n}{2} \inf \{ I_\beta(x) : x \geq \epsilon \} \right],$$

where

$$I_\beta(x) = c \coth(c) - 1 - \log \left( \frac{\sinh(c)}{c} \right) - \frac{\beta}{2} \left| \coth(c) - \frac{1}{c} \right|^2,$$

and  $c$  is the unique element of  $\mathbb{R}^+$  such that  $|x| = \coth(c) - \frac{1}{c}$ . It is shown in the appendix that  $I_\beta(x)$  is increasing for  $\beta < 3$ , and thus  $\inf \{ I_\beta(x) : x \geq \epsilon \} = I_\beta(\epsilon)$ . Moreover, there is a universal constant  $r > 0$  such that for  $\epsilon \in (0, 1)$ ,  $I_\beta(\epsilon) \geq \frac{\epsilon^2}{6} (1 - \frac{\beta}{3}) - r\epsilon^3$ . It follows that

$$\mathbb{P} \left[ \frac{\beta|\sigma^{(i)}|}{n} > \epsilon \right] \leq C \exp \left[ -\frac{n\epsilon^2}{12} \left( 1 - \frac{\beta}{3} \right) + nr\epsilon^3 \right].$$

Moving on to the error  $E'$ , it is true in general for  $x \in \mathbb{R}^n$  that  $\|xx^T\|_{HS} = |x|^2$ , and so

$$\mathbb{E}\|MM^T\|_{HS} = \mathbb{E}|M|^2 \leq 3$$

and

$$\mathbb{E}\|\sigma_i \sigma_i^T\|_{HS} = \mathbb{E}|\sigma_i|^2 = 1.$$

Estimating  $\mathbb{E}\|\frac{1}{n} \sum_{i=1}^n (3\sigma_i \sigma_i^T - Id)\|_{HS}$  is a bit more involved. First, recall that  $\|A\|_{HS} = \sqrt{\text{Tr}(AA^T)}$ , and so by the Cauchy-Schwarz inequality,

$$\mathbb{E}\left\|\frac{1}{n} \sum_{i=1}^n (3\sigma_i \sigma_i^T - Id)\right\|_{HS} \leq \frac{1}{n} \sqrt{\sum_{i,j=1}^n \mathbb{E} \text{Tr}[(3\sigma_i \sigma_i^T - Id)(3\sigma_j \sigma_j^T - Id)]}.$$

Now,

$$\mathbb{E} \text{Tr}[(3\sigma_i \sigma_i^T - Id)^2] = \mathbb{E}[9\text{Tr}(\sigma_i \sigma_i^T \sigma_i \sigma_i^T) - 6\text{Tr}(\sigma_i \sigma_i^T) + Id] = 9\mathbb{E}|\sigma_i|^4 - 6\mathbb{E}|\sigma_i|^2 + 3 = 6.$$

Similarly, for  $i \neq j$ ,

$$\mathbb{E} \text{Tr}[(3\sigma_i \sigma_i^T - Id)(3\sigma_j \sigma_j^T - Id)] = 9\mathbb{E}[\langle \sigma_i, \sigma_j \rangle^2] - 3.$$

Observe that

$$\begin{aligned} \mathbb{E}[\langle \sigma_1, \sigma_2 \rangle^2 | \{\sigma_i\}_{i \neq 1}] &= \sigma_2^T \mathbb{E}[\sigma_1 \sigma_1^T | \{\sigma_i\}_{i \neq 1}] \sigma_2 \\ &= \sigma_2^T \left( \frac{1}{Z_1} \int_{\mathbb{S}^2} \theta \theta^T \exp\left[\frac{\beta}{n} \langle \theta, \sigma^{(1)} \rangle\right] d\mu(\theta) \right) \sigma_2 \\ &= \sigma_2^T \left( \left[1 - \frac{2c \coth(c) - 2}{c^2}\right] P_i + \left[\frac{c \coth(c) - 1}{c^2}\right] P_i^\perp \right) \sigma_2, \end{aligned}$$

where we have made use of the computation of expression (5) carried out earlier, and again  $c = \frac{\beta|\sigma^{(1)}|}{n}$ ,  $P_i$  denotes orthogonal projection onto the span of  $\sigma^{(1)}$ , and  $P_i^\perp$  denotes orthogonal projection onto the orthogonal complement of the span of  $\sigma^{(1)}$ . Once again making use of the fact that  $c = o(1)$  with high probability, and so  $\coth(c) - \frac{1}{c} \approx \frac{c}{3} - \frac{c^3}{45}$ ,

$$\mathbb{E}[\langle \sigma_1, \sigma_2 \rangle^2 | \{\sigma_i\}_{i \neq 1}] \approx \sigma_2^T \left( \frac{1}{3} Id + \frac{2c^2}{45} P_i - \frac{c^2}{45} P_i^\perp \right) \sigma_2 = \frac{1}{3} - \frac{c^2}{45} + \frac{c^2}{15} \mathbb{E}[\sigma_2^T \sigma_1 \sigma_1^T \sigma_2 | \{\sigma_i\}_{i \neq 1}].$$

Taking expectation of both sides yields

$$\mathbb{E}[\langle \sigma_1, \sigma_2 \rangle^2] \approx \frac{1}{3} + \mathbb{E}\left[-\frac{c^2}{45} + \frac{c^2}{15} \langle \sigma_1, \sigma_2 \rangle^2\right],$$

so that

$$\mathbb{E} \text{Tr}[(3\sigma_i \sigma_i^T - Id)(3\sigma_j \sigma_j^T - Id)] \approx \mathbb{E}\left[-\frac{c^2}{5} + \frac{3c^2}{5} \langle \sigma_1, \sigma_2 \rangle^2\right].$$

The error incurred in this approximation (for each pair  $i \neq j$ ) is

$$\mathbb{E}\left|9\sigma_2^T \left(\left[\frac{2}{3} - \frac{2c \coth(c) - 2}{c^2} - \frac{2c^2}{45}\right] P_i + \left[\frac{c \coth(c) - 1}{c^2} - \frac{1}{3} + \frac{c^2}{45}\right] P_i^\perp\right) \sigma_2\right| \leq r_1 \mathbb{E} c^3,$$

where  $r_1$  is a universal constant.

Now,

$$\mathbb{E}c^2 = \frac{\beta^2}{n^2} \sum_{i,j>1} \mathbb{E} \langle \sigma_i, \sigma_j \rangle \leq \frac{\beta^2}{n^2} \left[ n - 1 + (n-1)(n-2) \frac{\beta}{n(3-\beta)} \right] \leq \frac{3\beta^2}{n(3-\beta)},$$

and one can then trivially also estimate that

$$\mathbb{E}c^3 \leq \frac{3\beta^3}{n(3-\beta)},$$

and so

$$\mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n (3\sigma_i \sigma_i^T - Id) \right\|_{HS} \leq \sqrt{\frac{6 + \frac{r_2(\beta^2 + \beta^3)}{(3-\beta)}}{n}}.$$

The remaining term of the error  $E'$  is  $E''$ , for which the remainder from Taylor's theorem also suffices:

$$\begin{aligned} \mathbb{E} \|E''\|_{HS} &\leq \frac{a^2}{n^2} \sum_{i=1}^n \mathbb{E} \left\{ \left\| \left[ \frac{2}{3} - \frac{2c \coth(c) - 2}{c^2} \right] P_i \right\|_{HS} + \left\| \left[ \frac{\coth(c)}{c} - \frac{1}{c^2} - \frac{1}{3} \right] P_i^\perp \right\|_{HS} \right. \\ &\quad \left. - \left\| \left[ \coth(c) - \frac{1}{c} - \frac{c}{3} \right] (r_i \sigma_i^T + \sigma_i r_i^T) \right\|_{HS} \right\} \\ &\leq \frac{c_1(3-\beta)\beta}{n^3} \sum_{i=1}^n \mathbb{E} |\sigma^{(i)}| \\ &\leq \frac{c_1 \sqrt{3(3-\beta)}\beta}{n^{3/2}}, \end{aligned}$$

for a universal constant  $c_1$ , using the facts that  $\|P_i\|_{HS}$ ,  $\|P_i^\perp\|_{HS}$  and  $\|r_i \sigma_i^T\|_{HS}$  are all bounded by  $\sqrt{2}$  or better and that  $\mathbb{E} |\sigma^{(i)}| \leq \sqrt{\frac{3n}{3-\beta}}$ .

The final error term from Theorem 9 is trivial:

$$\mathbb{E} |M' - M|^3 = \frac{a^3}{n^{3/2}} \mathbb{E} |\sigma'_I - \sigma_I| \leq \frac{8a^3}{n^{3/2}}.$$

Using the estimates above in the statement of the theorem yields

$$\begin{aligned} |\mathbb{E}g(M) - \mathbb{E}g(Z)| &\leq M_1(g) \left[ \sqrt{\frac{6 + \frac{r_2(\beta^2 + \beta^3)}{(3-\beta)}}{4n}} + \frac{3c_1}{\sqrt{4n(1 - \frac{\beta}{3})}} + \frac{7\beta}{(3-\beta)n} + \frac{2\beta}{(3-\beta)n^2} \right] \\ &\quad + M_1(g) \frac{3b}{\sqrt{3-\beta}} \sqrt{n} \left[ \epsilon^2 + C \exp \left( -\frac{n\epsilon^2}{12} \left( 1 - \frac{\beta}{3} \right) + nr\epsilon^3 \right) \right] \\ &\quad + M_2(g) \sqrt{\frac{2\pi(3-\beta)}{n}}, \end{aligned}$$

for  $g \in C^2(\mathbb{R}^3)$ . Finally choose  $\epsilon = \epsilon(n)$  such that  $\epsilon^2 = \frac{12 \log(n)}{n(1 - \frac{\beta}{3})}$ .



We may now conclude that if  $\beta < 3$ , then

$$\sup_{g: M_1(g), M_2(g) \leq 1} |\mathbb{E}g(M) - \mathbb{E}g(Z)| \leq \frac{c_\beta \log(n)}{\sqrt{n}}$$

for some constant  $c_\beta$  depending only on  $\beta$ .

## 4 The magnetization in the supercritical phase

In the ordered regime, where  $\beta$  is large, the spins tend to align. Indeed, it follows from the large deviations principle that  $|S_n|$  is close to  $\frac{k_2 n}{\beta}$  with high probability. Let

$$W := \sqrt{n} \left[ \frac{\beta^2}{n^2 k_2^2} \left| \sum_{j=1}^n \sigma_j \right|^2 - 1 \right]; \quad (7)$$

we show below that  $W$  satisfies a central limit theorem. Since the distribution of the magnetization  $\frac{1}{n} \sum_{j=1}^n \sigma_j$  is rotationally invariant, this gives a complete picture of the asymptotic behavior of the magnetization.

In order to obtain the central limit theorem, we apply the following version of Stein's abstract normal approximation theorem (see [16], pg. 35), essentially due to Rinott and Rotar ([15], Thm. 1.2).

**Theorem 10.** *Let  $h : \mathbb{R} \rightarrow \mathbb{R}$  be bounded with bounded derivative. Suppose that  $(W, W')$  is an exchangeable pair and let  $\mathcal{F}$  be a  $\sigma$ -field with respect to which  $W$  is measurable. Suppose further that there is  $\lambda > 0$  and an  $\mathcal{F}$ -measurable random variable  $E$  such that*

$$\mathbb{E}[W' - W | \mathcal{F}] = -\lambda W + E.$$

*Then if  $Z$  is a centered Gaussian random variable with variance  $\sigma^2$ ,*

$$|\mathbb{E}h(W) - \mathbb{E}h(Z)| \leq \sqrt{\frac{\pi}{2}} \frac{\|h\|_\infty \mathbb{E}|E|}{\lambda} + 2\|h\|_\infty \mathbb{E} \left| \sigma^2 - \frac{1}{2\lambda} \mathbb{E}[(W' - W)^2 | \mathcal{F}] \right| + \frac{\|h'\|_\infty \mathbb{E}|W' - W|^3}{4\lambda}.$$

To apply the theorem to  $W$  as defined above, construct an exchangeable pair  $(W, W')$  using the Gibbs sampler as before; that is, define  $W'$  by first replacing a randomly chosen spin in  $\{\sigma_i\}$  according to its conditional distribution given the rest of the spins. Then

$$\begin{aligned} \mathbb{E}[W' - W | \sigma] &= -\frac{\beta^2}{n^{5/2} k_2^2} \sum_{i=1}^n \left[ 2 \sum_{k \neq i} \langle \sigma_i, \sigma_k \rangle - \mathbb{E} \left[ 2 \sum_{k \neq i} \langle \sigma_i, \sigma_k \rangle \mid \{\sigma_j\}_{j \neq i} \right] \right] \\ &= -\frac{2\beta^2}{n^{5/2} k_2^2} \left( \left| \sum_{i=1}^n \sigma_i \right|^2 - n \right) + \frac{2\beta^2}{n^{5/2} k_2^2} \sum_{i=1}^n \left[ \coth \left( \frac{\beta |\sigma^{(i)}|}{n} \right) - \frac{n}{\beta |\sigma^{(i)}|} \right] |\sigma^{(i)}| \\ &= -\frac{2}{n} W - \frac{2}{\sqrt{n}} + \frac{2\beta^2}{n^{3/2} k_2^2} + \frac{2\beta^2}{n^{5/2} k_2^2} \sum_{i=1}^n \left[ \coth \left( \frac{\beta |\sigma^{(i)}|}{n} \right) - \frac{n}{\beta |\sigma^{(i)}|} \right] |\sigma^{(i)}|. \end{aligned}$$

For notational convenience, let  $g(x) := \coth(x) - \frac{1}{x}$ . Then observe that

$$\left| g\left(\frac{\beta|\sigma^{(i)}|}{n}\right) - g\left(\frac{\beta|S_n|}{n}\right) \right| \leq \|g'\|_\infty \left| \frac{\beta|\sigma^{(i)}|}{n} - \frac{\beta|S_n|}{n} \right| \leq \frac{\|g'\|_\infty \beta}{n},$$

since  $S_n - \sigma^{(i)} = \sigma_i$ , which has length 1. It follows that

$$\frac{2\beta^2}{n^{5/2}k_2^2} \sum_{i=1}^n \mathbb{E} \left[ \left| g\left(\frac{\beta|\sigma^{(i)}|}{n}\right) - g\left(\frac{\beta|S_n|}{n}\right) \right| |\sigma^{(i)}| \right] \leq \frac{2\|g'\|_\infty \beta^3}{n^{3/2}k_2^2},$$

since  $|\sigma^{(i)}| \leq n$ . Next, observe that

$$\frac{2\beta^2}{n^{5/2}k_2^2} \sum_{i=1}^n \mathbb{E} \left[ \left| g\left(\frac{\beta|S_n|}{n}\right) \right| \left| |\sigma^{(i)}| - |S_n| \right| \right] \leq \frac{2\|g\|_\infty \beta^2}{n^{3/2}k_2^2},$$

and so

$$\mathbb{E} [W' - W | \sigma] = -\frac{2}{n}W - \frac{2}{\sqrt{n}} + \frac{2\beta^2}{n^{3/2}k_2^2} g\left(\frac{\beta|S_n|}{n}\right) |S_n| + E_1, \quad (8)$$

where  $\mathbb{E}|E_1| \leq \frac{c_\beta}{n^{3/2}}$ .

We next approximate  $g\left(\frac{\beta|S_n|}{n}\right)$  by a first-order Taylor polynomial, making use of the LDP for  $|S_n|$ . We have that

$$\limsup_{n \rightarrow \infty} \frac{1}{n} P_{n,\beta} \left[ \left| \frac{|S_n|}{n} - \frac{k_2}{\beta} \right| \geq \epsilon \right] \leq - \inf_{|x| - \frac{k_2}{\beta} \geq \epsilon} I_\beta(x), \quad (9)$$

where

$$I_\beta(x) = \Phi_\beta(y) - \varphi(\beta), \quad \Phi_\beta(y) = y|x| + \log \left( \frac{y}{\sinh(y)} \right) - \frac{\beta}{2}|x|^2,$$

and  $y$  is uniquely defined by

$$\coth(y) - \frac{1}{y} = |x|.$$

Recall also that

$$\varphi(\beta) = \inf_{x \geq 0} \Phi_\beta(y) = \frac{k_2^2}{2\beta} + \log \left( \frac{k_2}{\sinh(k_2)} \right).$$

It was moreover shown in the appendix that  $|x| = \frac{k_2}{\beta}$  corresponding to  $y = k_2$  is the unique minimizing set for  $\Phi_\beta$ , and that  $\Phi_\beta(y)$  is decreasing as a function of  $|x|$  on  $\left[0, \frac{k_2}{\beta}\right]$  and increasing on  $\left[\frac{k_2}{\beta}, \infty\right)$ . This means in particular that

$$\inf_{|x| - \frac{k_2}{\beta} \geq \epsilon} I_\beta(x) = \min \left\{ I_\beta \left( y \left( \frac{k_2}{\beta} + \epsilon \right) \right), I_\beta \left( y \left( \frac{k_2}{\beta} - \epsilon \right) \right) \right\},$$

where by  $I_\beta(y(t))$  we mean the value that  $I_\beta(y)$  takes on for all  $x$  with  $|x| = t$  and  $y$  defined in terms of  $|x|$  as above.

Now, we know that  $\Phi_\beta(y)$  is minimized on  $|x| = \frac{k_2}{\beta}$ , so that  $\Phi'_\beta(k_2) = 0$ . It is shown in the appendix that  $\Phi''_\beta(k_2) > 0$ , so that there is a constant  $K_\beta$  such that

$$\inf_{||x| - \frac{k_2}{\beta}| \geq \epsilon} I_\beta(x) \geq K_\beta \epsilon^2,$$

and so

$$P_{n,\beta} \left[ \left| \frac{|S_n|}{n} - \frac{k_2}{\beta} \right| \geq \epsilon \right] \leq e^{-K_\beta n \epsilon^2}.$$

Applying this estimate then yields

$$\begin{aligned} \mathbb{E} \left| \frac{2\beta^2}{n^{3/2}k_2^2} \left[ g\left(\frac{\beta|S_n|}{n}\right) - g(k_2) - g'(k_2) \left(\frac{\beta|S_n|}{n} - k_2\right) \right] |S_n| \right| \\ \leq \frac{2\beta^2}{n^{3/2}k_2^2} \|g''\|_\infty \epsilon^2 \mathbb{E} \left| |S_n| \mathbb{1} \left( \left| \frac{\beta|S_n|}{n} - k_2 \right| \leq \epsilon \right) \right| \\ + \frac{2\beta^2}{n^{3/2}k_2^2} [2\|g\|_\infty + \|g'\|_\infty(\beta + k_2)] \mathbb{E} \left| |S_n| \mathbb{1} \left( \left| \frac{\beta|S_n|}{n} - k_2 \right| \geq \epsilon \right) \right| \\ \leq \frac{2\beta^2}{\sqrt{n}k_2^2} \left[ C\epsilon^2 + C'e^{-K_\beta n \epsilon^2} \right], \end{aligned}$$

where we have also used the trivial estimate  $|S_n| \leq n$  in the last line. Choosing  $\epsilon^2 = \frac{\log(n)}{K_\beta n}$  gives that

$$\mathbb{E} \left| \frac{2\beta^2}{n^{3/2}k_2^2} \left[ g\left(\frac{\beta|S_n|}{n}\right) - g(k_2) - g'(k_2) \left(\frac{\beta|S_n|}{n} - k_2\right) \right] |S_n| \right| \leq c_\beta \frac{\log(n)}{n^{3/2}},$$

for some constant  $c_\beta$  depending only on  $\beta$ .

Combining this estimate with (8) and recalling that  $g(k_2) = \frac{k_2}{\beta}$  gives that

$$\mathbb{E} [W' - W | \sigma] = -\frac{2}{n}W + \frac{2}{\sqrt{n}} \left[ \frac{\beta|S_n|}{nk_2} - 1 \right] + \frac{2\beta^2 g'(k_2)}{n^{3/2}k_2^2} \left( \frac{\beta|S_n|}{n} - k_2 \right) |S_n| + E_2, \quad (10)$$

where  $\mathbb{E}|E_2| \leq \frac{c_\beta \log(n)}{n^{3/2}}$ .

Now, observe that

$$|S_n| = \frac{nk_2}{\beta} \sqrt{1 + \frac{W}{\sqrt{n}}} = \frac{nk_2}{\beta} \left( 1 + \frac{W}{2\sqrt{n}} + E_3 \right),$$

where  $|E_3| \leq \frac{C|W|^2}{n}$ . This means that the second term of (10) is

$$\frac{W}{n} + \frac{2E_3}{\sqrt{n}},$$

and  $\mathbb{E} \left| \frac{2E_3}{\sqrt{n}} \right| \leq \frac{C}{n^{3/2}} \mathbb{E}|W|^2 \leq \frac{C \log(n)}{n^{3/2}}$ , using the LDP as above. Similarly,

$$\frac{2\beta^2 g'(k_2)}{n^{3/2}k_2^2} \mathbb{E} \left| \left( \frac{\beta|S_n|}{n} - k_2 \right) |S_n| - \frac{k_2 W}{2\sqrt{n}} |S_n| \right| \leq \frac{c_\beta}{n^{5/2}} \mathbb{E} [|W|^2 |S_n|] \leq \frac{c_\beta \log(n)}{n^{3/2}},$$

and

$$\frac{2\beta^2 g'(k_2)}{n^{3/2} k_2^2} \mathbb{E} \left| \frac{k_2 W}{2\sqrt{n}} |S_n| - \frac{\sqrt{n} k_2^2 W}{2\beta} \right| \leq \frac{2\beta^2 g'(k_2)}{n^{3/2} k_2^2} \mathbb{E} \left[ \frac{C k_2^2 |W|^2}{4\beta} \right] \leq \frac{c_\beta \log(n)}{n^{3/2}},$$

again using that  $\mathbb{E}|W|^2 \leq \log(n)$ . Combining these estimates with (10) yields

$$\mathbb{E} [W' - W | \sigma] = -\frac{(1 - \beta g'(k_2))}{n} W + E_4, \quad (11)$$

where again  $\mathbb{E}|E_4| \leq \frac{c_\beta \log(n)}{n^{3/2}}$ . Recall that it was shown in the appendix that  $\beta g'(k_2) = \beta \left( \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right) < 1$ , and so the approximate linear regression condition in Stein's abstract normal approximation theorem holds with  $\lambda = \frac{(1 - \beta g'(k_2))}{n}$ .

The next step is to compute  $\mathbb{E} [(W' - W)^2 | \sigma]$ . From the definition,

$$\begin{aligned} \mathbb{E} [(W' - W)^2 | \sigma] &= \frac{\beta^4}{n^4 k_2^4} \sum_{i=1}^n \mathbb{E} \left[ \left( 2 \sum_{j \neq i} \langle \sigma_i^* - \sigma_i, \sigma_j \rangle \right)^2 \middle| \sigma, I = i \right] \\ &= \frac{4\beta^4}{n^4 k_2^4} \sum_{i=1}^n \sum_{j, k \neq i} \mathbb{E} [\sigma_j^T (\sigma_i^* - \sigma_i) (\sigma_i^* - \sigma_i)^T \sigma_k | \sigma, I = i]. \end{aligned} \quad (12)$$

Now,  $\mathbb{E} [(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i]$  was already computed exactly in the  $\beta < 3$  case, and was found to be

$$\begin{aligned} \mathbb{E} [(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i] &= \left\{ \left[ 1 - \frac{2c_i \coth(c_i) - 2}{c_i^2} \right] P_i + \left[ \frac{\coth(c_i)}{c_i} - \frac{1}{c_i^2} \right] P_i^\perp \right. \\ &\quad \left. - \left[ \coth(c_i) - \frac{1}{c_i} \right] (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T \right\}, \end{aligned}$$

where  $c_i = \frac{\beta |\sigma^{(i)}|}{n}$ ,  $r_i = \frac{\sigma^{(i)}}{|\sigma^{(i)}|}$ , and  $P_i$  is orthogonal projection onto  $r_i$ .

Recall that

$$P_{n,\beta} \left[ \left| \frac{\beta |\sigma^{(i)}|}{n} - \frac{k_2(n-1)}{n} \right| \geq \epsilon \right] \leq e^{-K_\beta n \epsilon^2}$$

and that

$$\coth(k_2) - \frac{1}{k_2} = \frac{k_2}{\beta}.$$

Using this above,

$$\begin{aligned} \mathbb{E} [(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i] &= \left( 1 - \frac{2}{\beta} \right) P_i + \frac{1}{\beta} P_i^\perp - \frac{k_2}{\beta} (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T + E'_i \\ &= \frac{1}{\beta} Id + \left( 1 - \frac{3}{\beta} \right) P_i - \frac{k_2}{\beta} (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T + E'_i, \end{aligned} \quad (13)$$

where

$$E'_i = \left( \frac{g(c_i)}{c_i} - \frac{1}{\beta} \right) Id + \left( \frac{3g(c_i)}{c_i} - \frac{3}{\beta} \right) P_i - \left( g(c_i) - \frac{k_2}{\beta} \right) (r_i \sigma_i^T + \sigma_i r_i^T).$$

Ignoring the  $E'_i$  for the moment and putting the main term of (13) into (12) yields

$$\frac{4\beta^4}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \left[ \frac{1}{\beta} \langle \sigma_j, \sigma_k \rangle + \left(1 - \frac{3}{\beta}\right) \sigma_j^T P_i \sigma_k - \frac{k_2}{\beta} (\sigma_j^T r_i \sigma_i^T \sigma_k + \sigma_j^T \sigma_i r_i^T \sigma_k) + \sigma_j^T \sigma_i \sigma_i^T \sigma_k \right].$$

The first term is

$$\frac{4\beta^3}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \langle \sigma_j, \sigma_k \rangle = \frac{4\beta^3}{n^4 k_2^4} \sum_{i=1}^n |\sigma^{(i)}|^2.$$

For the second term, note that  $\sigma_j^T P_i \sigma_k = \text{Tr}(\sigma_k \sigma_j^T r_i r_i^T)$ , and so

$$\sum_{j,k \neq i} \sigma_j^T P_i \sigma_k = \text{Tr}(\sigma^{(i)} [\sigma^{(i)}]^T r_i r_i^T) = \langle \sigma^{(i)}, r_i \rangle^2 = |\sigma^{(i)}|^2$$

and thus

$$\frac{4\beta^4}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \left(1 - \frac{3}{\beta}\right) \sigma_j^T P_i \sigma_k = \frac{4\beta^4}{n^4 k_2^4} \left(1 - \frac{3}{\beta}\right) \sum_i |\sigma^{(i)}|^2.$$

Similarly, for the first half of the third term,

$$-\frac{4\beta^3}{n^4 k_2^3} \sum_i \sum_{j,k \neq i} \sigma_j^T r_i \sigma_i^T \sigma_k = -\frac{4\beta^3}{n^4 k_2^3} \sum_i |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle,$$

and the second half is the same. Finally,

$$\frac{4\beta^4}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \sigma_j^T \sigma_i \sigma_i^T \sigma_k = \frac{4\beta^4}{n^4 k_2^4} \sum_i \langle \sigma_i, \sigma^{(i)} \rangle^2;$$

all together,

$$\begin{aligned} \mathbb{E}[(W' - W)^2 | \sigma] &= \frac{4\beta^4}{n^4 k_2^4} \sum_i \left[ \left(1 - \frac{2}{\beta}\right) |\sigma^{(i)}|^2 - \frac{2k_2}{\beta} |\sigma^{(i)}| \langle \sigma_i, \sigma^{(i)} \rangle + \langle \sigma_i, \sigma^{(i)} \rangle^2 \right] \\ &\quad + \frac{4\beta^4}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \sigma_j^T E'_i \sigma_k. \end{aligned}$$

In order to apply Stein's theorem, one must recognize in this expression a deterministic part plus a mean zero part. With this motivation in mind, we write

$$\begin{aligned} \mathbb{E}[(W' - W)^2 | \sigma] &= \frac{4\beta^4}{n^3 k_2^4} \left[ 2 \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} - \frac{2n^2 k_2^4}{\beta^4} \right] + \frac{4\beta^4}{n^4 k_2^4} \sum_i \left(1 - \frac{2}{\beta}\right) \left( |\sigma^{(i)}|^2 - \frac{(n-1)^2 k_2^2}{\beta^2} \right) \\ &\quad + \frac{4\beta^4}{n^4 k_2^4} \sum_i \left[ -\frac{2k_2}{\beta} \left( |\sigma^{(i)}| \langle \sigma_i, \sigma^{(i)} \rangle - \frac{n^2 k_2^3}{\beta^3} \right) + \langle \sigma_i, \sigma^{(i)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right] \\ &\quad + \frac{4\beta^4}{n^4 k_2^4} \sum_i \sum_{j,k \neq i} \sigma_j^T E'_i \sigma_k, \end{aligned} \tag{14}$$

and define  $\sigma$  such that, to top order in  $n$ ,

$$\frac{4\beta^4}{n^3 k_2^4} \left[ 2 \left( 1 - \frac{2}{\beta} \right) \frac{(n-1)^2 k_2^2}{\beta^2} - \frac{2n^2 k_2^4}{\beta^4} \right] = 2\lambda\sigma^2,$$

for  $\lambda = \frac{1-\beta g'(k_2)}{n}$  as above. Note that the top order in  $n$  of the expression inside the parentheses can be simplified to

$$\begin{aligned} \frac{2n^2 k_2^2}{\beta^2} \left[ 1 - \frac{2}{\beta} - \frac{k_2^2}{\beta^2} \right] &= \frac{2n^2 k_2^2}{\beta^2} \left[ 1 - \frac{2 \left( \coth(k_2) - \frac{1}{k_2} \right)}{k_2} - \left( \coth(k_2) - \frac{1}{k_2} \right)^2 \right] \\ &= \frac{2n^2 k_2^2}{\beta^2} \left[ 1 - \frac{\cosh^2(k_2)}{\sinh^2(k_2)} + \frac{1}{k_2^2} \right] \\ &= \frac{2n^2 k_2^2}{\beta^2} \left[ \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right] > 0, \end{aligned}$$

so defining  $\sigma$  in this way does in fact yield a strictly positive value of  $\sigma^2$  which depends only on  $\beta$  and is independent of  $n$ .

Then to apply Stein's abstract normal approximation theorem, it is necessary to estimate the expected absolute value of each of the terms above (except the  $2\lambda\sigma^2$  part).

For the first term, it follows as before from the LDP for  $|\sigma^{(i)}|$  that

$$\mathbb{E} \left| |\sigma^{(i)}|^2 - \frac{(n-1)^2 k_2^2}{\beta^2} \right| \leq (n-1)^2 \left[ \epsilon + e^{-K_\beta(n-1)\epsilon^2} \right];$$

taking  $\epsilon = \sqrt{\frac{\log(n)}{K_\beta(n-1)}}$  shows that

$$\mathbb{E} \left| |\sigma^{(i)}|^2 - \frac{(n-1)^2 k_2^2}{\beta^2} \right| \leq c_\beta \sqrt{\log(n)} n^{3/2}.$$

Next, observe that

$$|\langle \sigma_i, \sigma^{(i)} \rangle| |\sigma^{(i)}| - \langle \sigma_i, S_n \rangle |S_n| \leq |\langle \sigma_i, \sigma^{(i)} \rangle| + |S_n| \leq 2n.$$

Moreover,

$$\frac{4\beta^4}{n^4 k_2^4} \mathbb{E} \left| \sum_i \frac{2k_2}{\beta} \left( |S_n| \langle \sigma_i, S_n \rangle - \frac{n^2 k_2^3}{\beta^3} \right) \right| = \frac{8\beta^3}{n^4 k_2^3} \mathbb{E} \left| |S_n|^3 - \frac{n^3 k_2^3}{\beta^3} \right| \leq \frac{c_\beta \sqrt{\log(n)}}{n^{3/2}}.$$

Now, using the same definitions for  $g, c_i, r_i$  and  $P_i$  as before,

$$\begin{aligned} \mathbb{E} \left[ \langle \sigma_i, \sigma^{(i)} \rangle^2 \right] &= \mathbb{E} \left[ \sum_{j,k \neq i} \sigma_j^T \mathbb{E} [\sigma_i \sigma_i^T | \{\sigma_\ell\}_{\ell \neq i}] \sigma_k \right] \\ &= \mathbb{E} \left[ \sum_{j,k \neq i} \sigma_j^T \left[ \left( 1 - \frac{3g(c_i)}{c_i} \right) P_i + \frac{g(c_i)}{c_i} Id \right] \sigma_k \right] = \mathbb{E} \left[ \left( 1 - \frac{2g(c_i)}{c_i} \right) |\sigma^{(i)}|^2 \right]; \end{aligned}$$

this explains the choice of constants in (14). Furthermore,

$$\begin{aligned}
& \mathbb{E} \left[ \sum_i \left( \langle \sigma_i, \sigma^{(i)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right)^2 \right] \\
&= n \mathbb{E} \left( \langle \sigma_1, \sigma^{(1)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right)^2 \\
&\quad + n(n-1) \mathbb{E} \left( \langle \sigma_1, \sigma^{(1)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right) \left( \langle \sigma_2, \sigma^{(2)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right). \tag{15}
\end{aligned}$$

The first term will simply be estimated by  $c_\beta n^5$ . For the second, first let  $\sigma^{(1,2)} := \sum_{j>2} \sigma_j$  and observe that

$$\left| \mathbb{E} \langle \sigma_1, \sigma^{(1)} \rangle^2 \langle \sigma_2, \sigma^{(2)} \rangle^2 - \mathbb{E} \langle \sigma_1, \sigma^{(1)} \rangle^2 \langle \sigma_2, \sigma^{(1,2)} \rangle^2 \right| \leq C n^3.$$

Now,

$$\begin{aligned}
\mathbb{E} \langle \sigma_1, \sigma^{(1)} \rangle^2 \langle \sigma_2, \sigma^{(1,2)} \rangle^2 &= \mathbb{E} \left[ \sum_{i,j>1} \sum_{k,\ell>2} \sigma_i^T \sigma_1 \sigma_1^T \sigma_j \sigma_k^T \sigma_2 \sigma_\ell^T \sigma_\ell \right] \\
&= \mathbb{E} \left[ \sum_{i,j>1} \sum_{k,\ell>2} \sigma_i^T \mathbb{E} [\sigma_1 \sigma_1^T | \{\sigma_m\}_{m>1}] \sigma_j \sigma_k^T \sigma_2 \sigma_\ell^T \sigma_\ell \right] \\
&= \mathbb{E} \left[ \left(1 - \frac{2g(c_1)}{c_1}\right) |\sigma^{(1)}|^2 \langle \sigma_2, \sigma^{(1,2)} \rangle^2 \right]
\end{aligned}$$

By the LDP for  $\sigma^{(1)}$ , we can replace  $\frac{g(c_1)}{c_1}$  by  $\frac{1}{\beta}$  and  $|\sigma^{(1)}|^2$  by  $\frac{(n-1)k_2}{\beta}$ , incurring an error of size  $c_\beta \sqrt{\log(n)} n^{7/2}$ . At this point we are left with

$$\mathbb{E} \left[ \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \langle \sigma_2, \sigma^{(1,2)} \rangle^2 \right].$$

We can now go back to  $\sigma^{(2)}$  instead of  $\sigma^{(1,2)}$  (with another loss of order  $n^3$ ), and therefore replace the last expression with

$$\mathbb{E} \left[ \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \left(1 - \frac{2g(c_2)}{c_2}\right) |\sigma^{(2)}|^2 \right],$$

(using the expression for  $\mathbb{E}[\langle \sigma_i, \sigma^{(i)} \rangle]$  obtained above). One final application of the LDP for  $\sigma^{(2)}$  now means that, with loss of the same order as before, this expression is equal to

$$\left(1 - \frac{2}{\beta}\right)^2 \frac{(n-1)^4 k_2^4}{\beta^4}.$$

Using these approximations in (15) now yields

$$\mathbb{E} \left[ \sum_i \left( \langle \sigma_i, \sigma^{(i)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right)^2 \right] \leq c_\beta \sqrt{\log(n)} n^{11/2},$$

and so

$$\frac{4\beta^4}{n^4 k_2^4} \mathbb{E} \left| \sum_i \left( \langle \sigma_i, \sigma^{(i)} \rangle^2 - \left(1 - \frac{2}{\beta}\right) \frac{(n-1)^2 k_2^2}{\beta^2} \right) \right| \leq c_\beta (\log(n))^{1/4} n^{-5/4}.$$

Exactly the same sorts of arguments using LDP for  $\sigma^{(i)}$  also imply that all the errors from the  $E'_i$  terms are smaller than those already accounted for.

Finally,

$$\mathbb{E}|W' - W|^3 = \frac{8\beta^6}{n^{9/2} k_2^6} \mathbb{E} \left| \sum_{j \neq I} \langle \sigma_I^* - \sigma_I, \sigma_j \rangle \right|^3 \leq \frac{8\beta^6}{n^{3/2} k_2^6}.$$

The following result is now a consequence of the bounds above together with Theorem 10.

**Theorem 11.** *Let  $W$  be the recentered, renormalized norm squared of the magnetization, as defined in (7). There is a constant  $c_\beta$  depending only on  $\beta > 3$  such that if  $Z$  is a centered Gaussian random variable with variance*

$$\sigma^2 := \frac{4\beta^2}{(1 - \beta g'(k_2)) k_2^2} \left[ \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right],$$

for  $g(x) = \coth(x) - \frac{1}{x}$ , then

$$\sup_{\substack{\|h\|_\infty \leq 1 \\ \|h'\|_\infty \leq 1}} \left| \mathbb{E}h(W) - \mathbb{E}h(Z) \right| \leq c_\beta \left( \frac{\log(n)}{n} \right)^{1/4}.$$

## 5 The critical temperature

In this section, we prove a nonnormal limit theorem for the squared-length of the total magnetization at the critical temperature  $\beta = 3$ . Since the magnetization is spherically symmetric, this provides the limiting picture in the critical case.

Recall that the LDP for  $|S_n|$  implies in particular that

$$\mathbb{P} \left[ \frac{3|S_n|}{n} > \epsilon \right] \leq C \exp \left[ -\frac{n}{2} \inf \{ I_3(x) : x \geq \epsilon \} \right],$$

where

$$I_3(x) = c \coth(c) - 1 - \log \left( \frac{\sinh(c)}{c} \right) - \frac{3}{2} \left| \coth(c) - \frac{1}{c} \right|^2,$$

and  $c$  is the unique element of  $\mathbb{R}^+$  such that  $|x| = \coth(c) - \frac{1}{c}$ . It is shown in the appendix that  $I_3(x)$  is increasing, and thus  $\inf \{ I_3(x) : x \geq \epsilon \} = I_3(\epsilon)$ . Moreover, there is a universal constant  $r > 0$  such that for  $\epsilon \in (0, 1)$ ,  $I_3(\epsilon) \geq r\epsilon^4$  (note in particular the difference from the subcritical case). It follows that

$$\mathbb{P} \left[ \frac{3|S_n|}{n} > \epsilon \right] \leq C \exp [-cn\epsilon^4].$$



for some constant  $c > 0$ , and so

$$\mathbb{E} \left[ \frac{3|S_n|}{n} \right] \leq \epsilon + 3C \exp [-cn\epsilon^4].$$

Choosing  $\epsilon^4 = \frac{\log(n)}{cn}$  shows that  $\mathbb{E}[|S_n|] \leq \frac{C^4 \sqrt{\log(n)}}{n^{3/4}}$ . This at least suggests what turns out to be the correct normalization for the magnetization; below, we prove a nonnormal limit theorem for  $W := \frac{c_3}{n^{3/2}} \sum_{i,j=1}^n \langle \sigma_i, \sigma_j \rangle$ , for a particular choice of  $c_3$  (independent of  $n$ ). Indeed, one can use a modification of the argument given in the beginning of section 3 to show that

$$\mathbb{E}|S_n|^2 = n + \mathbb{E} \left[ |S_n|^2 - \frac{|S_n|^4}{5n^2} - \frac{2|S_n|^2}{n} + \frac{2 \cdot 3^5 |S_n|^6}{945n^4} + \text{lower order terms} \right],$$

from which it eventually follows that, to top order in  $n$ , there is a  $c_3$  such that

$$\mathbb{E}|S_n|^2 = \frac{n^{3/2}}{c_3} \quad \mathbb{E}|S_n|^4 = 5n^3.$$

The proof of the limit theorem for  $W$  as defined above is essentially via the so-called “density approach” to Stein’s method introduced by Stein, Diaconis, Holmes and Reinert [17]; see also the recent work of Chatterjee and Shao [3], with an application to the magnetization of the mean-field Ising model. The following theorem provides the framework we use for the approximation; the proof is given in Section 6.2 of the appendix.

**Theorem 12.** *Let  $(W, W')$  be an exchangeable pair of positive random variables. Suppose there exists a  $\sigma$ -field  $\mathcal{F} \supseteq \sigma(W)$  and  $k > 0$  deterministic such that*

$$\mathbb{E}[W' - W | \mathcal{F}] = 3k(1 - cW^2) + E$$

and

$$\mathbb{E}[(W' - W)^2 | \mathcal{F}] = kW + E'.$$

Let  $X$  have density

$$p(t) = \begin{cases} \frac{1}{2} x^5 e^{-\frac{ct^2}{2}} & t \geq 0; \\ 0 & t < 0. \end{cases}$$

Then there are constants  $C_1, C_2, C_3$  depending only on  $c$  such that for all  $h \in C^2(\mathbb{R})$ ,

$$\begin{aligned} |\mathbb{E}h(W) - \mathbb{E}h(X)| &\leq \frac{C_1 \|h\|_\infty}{k} \mathbb{E}|E| + \left( \frac{C_2 (\|h\|_\infty + \|h'\|_\infty)}{k} \right) \mathbb{E}|E'| \\ &\quad + \left( \frac{C_3 (\|h\|_\infty + \|h'\|_\infty + \|h''\|_\infty)}{k} \right) \mathbb{E}|W' - W|^3. \end{aligned}$$

Within this framework, we proceed as before: let  $W := \frac{c_3}{n^{3/2}} \sum_{i,j=1}^n \langle \sigma_i, \sigma_j \rangle$ , and make an exchangeable pair  $(W, W')$  by replacing a random spin using the Gibbs sampler. Then, as in the supercritical case,

$$\begin{aligned} \mathbb{E}[W' - W | \sigma] &= -\frac{c_3}{n^{5/2}} \sum_{i=1}^n \left[ 2 \sum_{k \neq i} \langle \sigma_i, \sigma_k \rangle - \mathbb{E} \left[ 2 \sum_{k \neq i} \langle \sigma_i, \sigma_k \rangle \mid \{\sigma_j\}_{j \neq i} \right] \right] \\ &= -\frac{2}{n} W + \frac{2c_3}{n^{3/2}} + \frac{2c_3}{n^{5/2}} \sum_{i=1}^n g \left( \frac{3|\sigma^{(i)}|}{n} \right) |\sigma^{(i)}|, \end{aligned} \tag{16}$$

again using the notation  $g(x) = \coth(x) - \frac{1}{x}$ . Now, near zero,  $g(x) = \frac{x}{3} - \frac{x^3}{45} + O(x^5)$ . Using this above,

$$\sum_{i=1}^n g\left(\frac{3|\sigma^{(i)}|}{n}\right) |\sigma^{(i)}| = \sum_{i=1}^n \left[ \frac{|\sigma^{(i)}|^2}{n} - \frac{|\sigma^{(i)}|^4}{5n^3} + O\left(\frac{|\sigma^{(i)}|^6}{n^5}\right) \right].$$

Note that

$$\frac{1}{n} \sum_{i=1}^n |\sigma^{(i)}|^2 = \sum_{j,k} \langle \sigma_j, \sigma_k \rangle - \frac{2}{n} \sum_{i,j} \langle \sigma_i, \sigma_j \rangle + 1 = \frac{n^{3/2}W}{c_3} - \frac{2\sqrt{n}W}{c_3} + 1.$$

Similarly,

$$-\frac{1}{5n^3} \sum_{i=1}^n |\sigma^{(i)}|^4 = -\frac{nW^2}{5c_3^2} + \frac{4W^2}{5c_3^2} - \frac{4 \sum_i \langle \sigma_i, S_n \rangle^2}{5n^3} - \frac{2W}{5c_3\sqrt{n}} + \frac{W}{5n^{3/2}c_3} + \frac{1}{5n^2}.$$

Using these expressions in (16) yields

$$\mathbb{E} [W' - W | \sigma] = \frac{2c_3}{n^{3/2}} - \frac{2W^2}{5c_3n^{3/2}} + E,$$

where

$$E = -\frac{4W}{n^2} + \frac{8W^2}{5c_3n^{5/2}} + \frac{CW^3}{n^2c_3^2} + \frac{R(\sigma)}{n^{5/2}},$$

$C$  is a universal constant, and furthermore,  $R(\sigma) \leq C$  almost surely. Note in particular the cancellation of the  $\frac{2}{n}W$  terms, which is the crucial difference from the subcritical case, and the reason that the limiting distribution of the magnetization is not Gaussian for  $\beta = 3$ .

Recall that the LDP for  $\mu_{\sigma,n}$  gives us that  $\mathbb{E}W, \mathbb{E}W^2, \mathbb{E}W^3 \leq \log(n)$ , and so it follows that  $\mathbb{E}|E| \leq \frac{C \log(n)}{n^2}$ .

To apply Theorem 12, we take  $k = \frac{2c_3}{3n^{3/2}}$  and  $c = \frac{1}{5c_3}$ .

The next step is to compute  $\mathbb{E} [(W' - W)^2 | \sigma]$ . From the definition as before,

$$\mathbb{E} [(W' - W)^2 | \sigma] = \frac{c_3^2}{n^4} \sum_{i=1}^n \sum_{j,k \neq i} \mathbb{E} [\sigma_j^T (\sigma_i^* - \sigma_i) (\sigma_i^* - \sigma_i)^T \sigma_k | \sigma, I = i]. \quad (17)$$

Now,  $\mathbb{E} [(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i]$  was already computed exactly in the  $\beta < 3$  case, and was found to be

$$\begin{aligned} \mathbb{E} [(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i] = & \left\{ \left[ 1 - \frac{2c_i \coth(c_i) - 2}{c_i^2} \right] P_i + \left[ \frac{\coth(c_i)}{c_i} - \frac{1}{c_i^2} \right] P_i^\perp \right. \\ & \left. - \left[ \coth(c_i) - \frac{1}{c_i} \right] (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T \right\}, \end{aligned}$$

where  $c_i = \frac{\beta|\sigma^{(i)}|}{n}$ ,  $r_i = \frac{\sigma^{(i)}}{|\sigma^{(i)}|}$ ,  $P_i$  is orthogonal projection onto  $r_i$ , and  $P_i^\perp$  is orthogonal projection onto the orthogonal complement of  $r_i$ .

Now, recall that  $g(x) = \coth(x) - \frac{1}{x} \approx \frac{x}{3}$  for small  $x$ . Using this above,

$$\mathbb{E}[(\sigma_i^* - \sigma_i)(\sigma_i^* - \sigma_i)^T | \sigma, I = i] = \frac{1}{3} Id - \frac{c_i}{3} (r_i \sigma_i^T + \sigma_i r_i^T) + \sigma_i \sigma_i^T + E'_i, \quad (18)$$

where

$$E'_i = \left( \frac{g(c_i)}{c_i} - \frac{1}{3} \right) Id - \left( g(c_i) - \frac{c_i}{3} \right) (r_i \sigma_i^T + \sigma_i r_i^T).$$

Ignoring the  $E'_i$  for the moment and putting the main term of (18) into (17) yields

$$\frac{c_3^2}{n^4} \sum_i \sum_{j, k \neq i} \left[ \frac{1}{3} \langle \sigma_j, \sigma_k \rangle - \frac{c_i}{3} (\sigma_j^T r_i \sigma_i^T \sigma_k + \sigma_j^T \sigma_i r_i^T \sigma_k) + \sigma_j^T \sigma_i \sigma_i^T \sigma_k \right].$$

The first term is

$$\frac{c_3^2}{3n^4} \sum_i \sum_{j, k \neq i} \langle \sigma_j, \sigma_k \rangle = \frac{c_3^2}{3n^4} \sum_{i=1}^n |\sigma^{(i)}|^2.$$

The first half of the second term is

$$-\frac{c_3^2}{3n^4} \sum_i \sum_{j, k \neq i} c_i \sigma_j^T r_i \sigma_i^T \sigma_k = -\frac{c_3^2}{3n^4} \sum_i c_i |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle = -\frac{c_3^2}{n^5} \sum_i |\sigma^{(i)}|^2 \langle \sigma^{(i)}, \sigma_i \rangle,$$

and the second half is the same. Finally,

$$\frac{c_3^2}{n^4} \sum_i \sum_{j, k \neq i} \sigma_j^T \sigma_i \sigma_i^T \sigma_k = \frac{c_3^2}{n^4} \sum_i \langle \sigma_i, \sigma^{(i)} \rangle^2;$$

all together,

$$\begin{aligned} \mathbb{E}[(W' - W)^2 | \sigma] &= \frac{c_3^2}{n^4} \sum_i \left[ \frac{1}{3} |\sigma^{(i)}|^2 - \frac{2}{n} |\sigma^{(i)}|^2 \langle \sigma_i, \sigma^{(i)} \rangle + \langle \sigma_i, \sigma^{(i)} \rangle^2 \right] \\ &\quad + \frac{c_3^2}{n^4} \sum_i \sum_{j, k \neq i} \sigma_j^T E'_i \sigma_k \\ &= \frac{c_3^2}{n^4} \sum_i \left[ \frac{2}{3} |\sigma^{(i)}|^2 - \frac{2}{n} |\sigma^{(i)}|^2 \langle \sigma_i, \sigma^{(i)} \rangle \right] + \frac{c_3^2}{n^4} \sum_i \sum_{j, k \neq i} \sigma_j^T E'_i \sigma_k \\ &= \frac{2c_3^2}{3n^3} \left( |S_n|^2 - \frac{|S_n|^2}{n} + 1 \right) - \frac{2c_3^2}{n^5} \sum_i |\sigma^{(i)}|^2 \langle \sigma_i, \sigma^{(i)} \rangle + \frac{c_3^2}{n^4} \sum_i \sum_{j, k \neq i} \sigma_j^T E'_i \sigma_k, \end{aligned}$$

where the computation for  $\mathbb{E}[\langle \sigma_i, \sigma^{(i)} \rangle^2]$  from the supercritical case has been used. Recall that the main term should be  $\frac{2c_3 W}{3n^{3/2}}$  and indeed it is. It is a routine collection of arguments very similar to those in the previous sections to show that the remaining terms are bounded in expectation by  $\frac{C \log(n)}{n^2}$ .

Finally,

$$\begin{aligned}\mathbb{E}|W' - W|^3 &= \frac{8c_3^3}{n^{9/2}} \mathbb{E} \left| \sum_{j \neq I} \langle \sigma_I^* - \sigma_I, \sigma_j \rangle \right|^3 = \frac{8c_3^3}{n^{9/2}} \mathbb{E} |\langle \sigma_I^* - \sigma_I, S_n - \sigma_I \rangle|^3 \\ &\leq \frac{8c_3^3}{n^{9/2}} [8\mathbb{E}|S_n|^3 + 8] \leq \frac{C \log(n)}{n^{9/4}}.\end{aligned}$$

Using these estimates and the choices of  $k$  and  $c$  in Theorem 12 yields the following

**Theorem 13.** *At the critical temperature  $\beta = 3$ , let  $W := \frac{c_3 |S_n|^2}{n^{3/2}}$ , where  $c_3$  is such that  $\mathbb{E}W = 1$ . Let  $X$  have density*

$$p(t) = \begin{cases} \frac{1}{z} t^5 e^{-3ct^2} & t \geq 0; \\ 0 & t < 0, \end{cases}$$

where  $c = \frac{1}{5c_3}$  and  $z$  is a normalizing factor. Then there is a universal constant  $C$  such that

$$\sup_{\substack{\|h\|_\infty \leq 1, \|h'\|_\infty \leq 1 \\ \|h''\|_\infty \leq 1}} |\mathbb{E}h(W) - \mathbb{E}h(X)| \leq \frac{C \log(n)}{\sqrt{n}}.$$

## 6 Appendix

### 6.1 Calculus of $\Phi_\beta$

**Lemma 14.** *If  $\beta \leq 3$ , then*

$$\inf_{x \geq 0} \left\{ \log \left( \frac{x}{\sinh(x)} \right) + x \left( \coth(x) - \frac{1}{x} \right) - \frac{\beta}{2} \left( \coth(x) - \frac{1}{x} \right)^2 \right\} = 0,$$

achieved only at  $x = 0$ .

*Proof.* We show first that the expression to be minimized is increasing. Differentiating the expression in question yields

$$\begin{aligned}& \left[ \frac{\sinh(x)}{x} \right] \left[ \frac{\sinh(x) - x \cosh(x)}{\sinh^2(x)} \right] + \left[ \coth(x) - \frac{1}{x} \right] + x \left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \\ & \quad - \beta \left[ \coth(x) - \frac{1}{x} \right] \left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \\ &= \left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \left[ x - \beta \left( \coth(x) - \frac{1}{x} \right) \right].\end{aligned}$$

Expanding  $\sinh(x)$  in a Taylor series,

$$\sinh^2(x) = \left( x + \sum_{n=1}^{\infty} \frac{x^{2n+1}}{(2n+1)!} \right)^2 > x^2.$$

The problem is therefore reduced to showing that

$$x - \beta \left( \coth(x) - \frac{1}{x} \right) > 0,$$

or alternatively,

$$\beta < \frac{x^2}{x \coth(x) - 1}.$$

Clearly showing this for  $\beta = 3$  suffices to prove the lemma. Rearranging yet again, this is equivalent to showing that

$$\coth(x) - \frac{1}{x} < \frac{x}{3}.$$

Expanding  $\coth(x)$  in terms of  $e^{2x}$  and rearranging terms, this is furthermore equivalent to showing that

$$\left( 1 - x + \frac{x^2}{3} \right) e^{2x} > 1 + x + \frac{x^2}{3}.$$

Expanding  $e^{2x}$  in a Taylor series, the left-hand side of the inequality above is given by

$$\begin{aligned} 1 + x + \frac{x^2}{3} + \sum_{n=3}^{\infty} x^n \left[ \frac{2^n}{n!} - \frac{2^{n-1}}{(n-1)!} + \frac{2^{n-2}}{3(n-2)!} \right] \\ = 1 + x + \frac{x^2}{3} + \sum_{n=3}^{\infty} \frac{2^{n-2} x^n}{3n!} \left[ \left( n - \frac{7}{2} \right)^2 - \frac{1}{4} \right]. \end{aligned}$$

It is easy to see that the  $n = 3$  and  $n = 4$  terms in the power series above are zero and that the rest are all positive, thus completing the proof that the expression to be minimized is increasing. Moreover, recall that  $\lim_{x \rightarrow 0} \coth(x) - \frac{1}{x} = 0$  and  $\lim_{x \rightarrow 0} \frac{x}{\sinh(x)} = 1$ , so

$$\lim_{x \rightarrow 0} \left\{ \log \left( \frac{x}{\sinh(x)} \right) + x \left( \coth(x) - \frac{1}{x} \right) - \frac{\beta}{2} \left( \coth(x) - \frac{1}{x} \right)^2 \right\} = 0.$$

□

**Lemma 15.** *For  $\beta > 3$ , there is a unique value of  $x \in (0, \infty)$  which minimizes*

$$\log \left( \frac{x}{\sinh(x)} \right) + x \left( \coth(x) - \frac{1}{x} \right) - \frac{\beta}{2} \left( \coth(x) - \frac{1}{x} \right)^2$$

*over  $[0, \infty)$ .*

*Proof.* From the previous proof, we have that the derivative of the expression to be minimized is

$$\left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \left[ x - \beta \left( \coth(x) - \frac{1}{x} \right) \right] \sim \frac{(3 - \beta)x}{9},$$

for  $x$  near zero. For  $\beta > 3$ , it follows that  $x = 0$  is a local maximum of the expression on  $[0, \infty)$ . As  $x$  tends to infinity, the expression to be minimized is asymptotic to  $\log(x)$ , and

there is therefore at least one interior minimum. Since  $\frac{1}{x^2} - \frac{1}{\sinh^2(x)} > 0$ , it must be the case that at this interior minimum,

$$x - \beta \left( \coth(x) - \frac{1}{x} \right) = 0;$$

that is,

$$\beta = \frac{x}{\coth(x) - \frac{1}{x}}.$$

In fact, the function  $g(x) = \frac{x}{\coth(x) - \frac{1}{x}}$  is strictly increasing on  $(0, \infty)$ , and this equation thus uniquely determines  $x$  in terms of  $\beta$ . First observe that

$$g'(x) = \frac{\coth(x) - \frac{2}{x} + \frac{x}{\sinh^2(x)}}{\left(\coth(x) - \frac{1}{x}\right)^2},$$

and it thus suffices to show that

$$\coth(x) - \frac{2}{x} + \frac{x}{\sinh^2(x)} > 0$$

for  $x > 0$ ; multiplying through by  $x \sinh^2(x)$ , one could equivalently show that

$$x \sinh(x) \cosh(x) + x^2 - 2 \sinh^2(x) > 0.$$

Using the identities  $\sinh(x) \cosh(x) = \frac{\sinh(2x)}{2}$  and  $\sinh^2(x) = \frac{\cosh(2x) - 1}{2}$ , this is equivalent to showing that

$$\frac{x}{2} \sinh(2x) + x^2 - \cosh(2x) + 1 > 0.$$

Expanding the left-hand side in Taylor series yields

$$\sum_{n=2}^{\infty} x^{2n} \left[ \frac{2^{2n-1}}{2(2n-1)!} - \frac{2^{2n}}{(2n)!} \right] = \sum_{n=3}^{\infty} \frac{x^{2n} 2^{2n-2}}{(2n)!} [2n-4],$$

all of whose terms are indeed positive. □

**Lemma 16.** *Let  $k_2$  denote the unique value of  $x \in (0, \infty)$  with*

$$x - \beta \left( \coth(x) - \frac{1}{x} \right) = 0.$$

*Then*

$$\beta \left( \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right) < 1.$$

*In particular, if*

$$\Phi_\beta(x) := \log \left( \frac{x}{\sinh(x)} \right) + x \left( \coth(x) - \frac{1}{x} \right) - \frac{\beta}{2} \left( \coth(x) - \frac{1}{x} \right)^2,$$

*then  $\Phi'_\beta(k_2) = 0$  and  $\Phi''_\beta(k_2) > 0$ .*

*Proof.* Let

$$f(x) := x - \beta \left( \coth(x) - \frac{1}{x} \right),$$

so that  $f(k_2) = 0$ ; as was shown in the previous proof, this uniquely defines  $k_2$  in terms of  $\beta$ . Moreover, it was also shown that  $\lim_{x \rightarrow 0} f(x) = 0$ ,  $\lim_{x \rightarrow \infty} f(x) = \infty$ , and  $\lim_{x \rightarrow 0} f'(x) < 0$ . That is,  $f$  is initially decreasing from 0, and then becomes increasing eventually, crossing the  $x$ -axis exactly once in  $(0, \infty)$ . It must therefore be that there is an  $x < k_2$  such that  $f'(x) = 0$ . Now,

$$f'(x) = 1 - \beta \left( \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right).$$

In fact,  $g(x) := \frac{1}{x^2} - \frac{1}{\sinh^2(x)}$  is decreasing on  $(0, \infty)$ : observe first that

$$g'(x) = 2 \coth(x) \operatorname{csch}^2(x) - \frac{2}{x^3},$$

and so the claim is true if  $\coth(x) \operatorname{csch}^2(x) < x^{-3}$ . By the definitions of the hyperbolic trigonometric functions, this is equivalent to

$$4x^3(e^{4x} + e^{2x}) < (e^{2x} - 1)^3.$$

Expanding in power series, this is equivalent to

$$\sum_{n=3}^{\infty} \frac{4(4^{n-3} + 2^{n-3})}{(n-3)!} x^n < \left( \sum_{n=1}^{\infty} \frac{(2x)^n}{n!} \right)^3 = \sum_{n=3}^{\infty} \left( \sum_{\substack{i,j,k \geq 1 \\ i+j+k=n}} \frac{2^n}{i!j!k!} \right) x^n.$$

Letting  $\alpha := i - 1$ ,  $\beta := j - 1$ , and  $\gamma = k - 1$ , the coefficient of  $x^n$  on the right-hand side is

$$\frac{2^n}{(n-3)!} \sum_{\substack{\alpha, \beta, \gamma \geq 0 \\ \alpha + \beta + \gamma = n-3}} \binom{n-3}{\alpha, \beta, \gamma} = \frac{2^n}{(n-3)!} 3^{n-3}.$$

It is now easy to see that the coefficient of  $x^n$  on the right-hand side is smaller than the one on the left for each  $n \geq 3$ , and so it is in fact true that  $g(x) := \frac{1}{x^2} - \frac{1}{\sinh^2(x)}$  is decreasing on  $(0, \infty)$ . It follows that  $f'(x)$  is increasing on  $(0, \infty)$ , and so the previously identified  $x < k_2$  such that  $f'(x) = 0$  is in fact the only zero of  $f'$ , and  $f'(k_2) > 0$ .

Now, recall from the proof of the previous lemma that

$$\Phi'_\beta(x) = \left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \left[ x - \beta \left( \coth(x) - \frac{1}{x} \right) \right].$$

The value  $k_2$  was in fact determined by the fact that  $\Phi'_\beta(k_2) = 0$ . Moreover,

$$\begin{aligned} \Phi''_\beta(x) &= \left[ \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right] \left[ 1 - \beta \left( \frac{1}{x^2} - \frac{1}{\sinh^2(x)} \right) \right] \\ &\quad + \left[ 2 \coth(x) \operatorname{csch}^2(x) - \frac{2}{x^3} \right] \left[ x - \beta \left( \coth(x) - \frac{1}{x} \right) \right], \end{aligned}$$

and so

$$\Phi''_{\beta}(k_2) = \left[ \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right] \left[ 1 - \beta \left( \frac{1}{k_2^2} - \frac{1}{\sinh^2(k_2)} \right) \right] > 0$$

□

## 6.2 Proof of Theorem 12

This section is devoted to the proof of the abstract approximation theorem used in Section 5. The following theorem is the starting point.

**Theorem 17.** *Let  $Y$  be a positive random variable. Then  $Y$  has density*

$$p(t) = \begin{cases} \frac{1}{z} t^5 e^{-3ct^2} & t \geq 0; \\ 0 & t < 0. \end{cases}$$

if and only if

$$\mathbb{E}[Y f'(Y) + 6(1 - cY^2)f(Y)] = 0 \quad (19)$$

for all  $f \in C^1((0, \infty))$  such that  $\int_0^\infty f(t) t^5 e^{-3ct^2} dt < \infty$ .

*Proof.* If  $Y$  has the density above, then the fact that  $Y$  satisfies (19) is just integration by parts.

For the reverse implication, one must solve the so-called Stein equation; i.e., given  $h : (0, \infty) \rightarrow \mathbb{R}$ , find  $f = f_h$  such that

$$t f'(t) + 6(1 - ct^2)f(t) = h(t) - \mathbb{E}h(X),$$

where  $X$  has the density above. The solution  $f$  is given by

$$\begin{aligned} f(t) &= \frac{1}{tp(t)} \int_0^t [h(s) - \mathbb{E}h(X)] p(s) ds \\ &= -\frac{1}{tp(t)} \int_t^\infty [h(s) - \mathbb{E}h(X)] p(s) ds, \end{aligned}$$

where  $p(s) := \frac{s^5}{z} e^{-3cs^2}$ . Observe that

$$\frac{d}{dt} [t f(t) p(t)] = [f(t) + t f'(t)] p(t) + t f(t) p'(t) = [h(t) - \mathbb{E}h(X)] p(t),$$

so that

$$h(t) - \mathbb{E}h(X) = f(t) + t f'(t) + \frac{t f(t) p'(t)}{p(t)} = 6(1 - ct^2)f(t) + t f'(t).$$

Here we have made use of the fact, frequently used below, that

$$\frac{tp'(t)}{p(t)} = 5 - 6ct^2.$$

It is shown in the next lemma that  $f$  and  $f'$  are both bounded, and so if  $Y$  satisfies (19), then if  $h$  is given and  $f$  solves the Stein equation,

$$\mathbb{E}h(Y) - \mathbb{E}h(X) = \mathbb{E}[Y f'(Y) + 6(1 - cY^2)f(Y)] = 0,$$

and so  $Y \stackrel{d}{=} X$ .

□



The next lemma gives the required boundedness properties of  $f_h$ .

**Lemma 18.** *Suppose  $f = f_h$  is as defined above. Then*

- (a)  $\|f_h\|_\infty \leq 5\|h\|_\infty$ .
- (b)  $\|f'_h\|_\infty \leq 42\sqrt{c}\|h\|_\infty + 3\|h'\|_\infty$ .
- (c)  $\|f''_h\|_\infty \leq C_1\|h\|_\infty + C_2\|h'\|_\infty + C_3\|h''\|_\infty$ , where  $C_1, C_2, C_3$  are constants depending only on  $c$ .

*Proof.* (a) By the first expression for  $f_h$ , if  $t \leq t_o := \sqrt{\frac{5}{6c}}$ , then

$$f(t) \leq \frac{2\|h\|_\infty}{tp(t)} \left( \int_0^t p(s)ds \right) \leq \frac{\|h\|_\infty t^5}{3zp(t)} \leq \frac{e^{5/2}\|h\|_\infty}{3} \leq 5\|h\|_\infty.$$

By the second expression for  $f_h$ ,

$$|f(t)| \leq \frac{2\|h\|_\infty \mathbb{P}[X \geq t]}{tp(t)}.$$

It is easy to show directly that  $\mathbb{P}[X \geq t] \leq \frac{p(t)}{6ct} \left( 1 + \frac{2}{3ct^2} + \frac{2}{9c^2t^4} \right)$ , and so

$$|f(t)| \leq \frac{2\|h\|_\infty}{6ct^2} \left( 1 + \frac{2}{3ct^2} + \frac{2}{9c^2t^4} \right) \leq \frac{84\|h\|_\infty}{125}$$

for  $t \geq t_o$ . This completes the proof.

(b) Recall that, because  $f$  solves the Stein equation,

$$tf'(t) = 6f(t)(ct^2 - 1) + h(t) - \mathbb{E}h(X).$$

For  $t \leq t_o$ , observe that

$$\begin{aligned} h(t) - \mathbb{E}h(X) - 6f(t) &= h(t) - \mathbb{E}h(X) - \frac{6}{tp(t)} \int_0^t [h(s) - \mathbb{E}h(X)]p(s)ds \\ &= \frac{6}{tp(t)} \int_0^t \left( [h(t) - \mathbb{E}h(X)] \frac{s^5 p(t)}{t^5} - [h(s) - \mathbb{E}h(X)]p(s) \right) ds. \end{aligned}$$

Now,

$$\begin{aligned} &\left| \frac{1}{tp(t)} \int_0^t [h(t) - \mathbb{E}h(X)] \left( \frac{s^5 p(t)}{t^5} - p(s) \right) ds \right| \\ &\leq \frac{2\|h\|_\infty}{tp(t)} \int_0^t \left| 1 - \frac{s^5 p(t)}{t^5 p(s)} \right| p(s) ds = \frac{2\|h\|_\infty}{tp(t)} \int_0^t \left| 1 - e^{3c(s^2 - t^2)} \right| p(s) ds \\ &\leq 2\|h\|_\infty ct^2, \end{aligned}$$

making use of the fact that  $p(s) \leq p(t)$  in this range. Also,

$$\begin{aligned} \left| \frac{1}{tp(t)} \int_0^t ([h(t) - \mathbb{E}h(X)] - [h(s) - \mathbb{E}h(X)]) p(s) ds \right| \\ \leq \frac{\|h'\|_\infty}{tp(t)} \int_0^t (t-s)p(s) ds \leq \frac{\|h'\|_\infty t}{2}, \end{aligned}$$

so that for  $t \leq t_o$ ,

$$\frac{1}{t} |h(t) - \mathbb{E}h(X) - 6f(t)| \leq 12\|h\|_\infty ct_o + 3\|h'\|_\infty,$$

and thus

$$\begin{aligned} |f'(t)| &\leq 6ct_o\|f\|_\infty + 12\|h\|_\infty ct_o + 3\|h'\|_\infty \\ &\leq 42ct_o\|h\|_\infty + 3\|h'\|_\infty. \end{aligned}$$

If  $t \geq t_o$ , then

$$|f'(t)| \leq 6ct|f(t)| + \frac{6\|f\|_\infty + 2\|h\|_\infty}{t_o}.$$

By the second expression for  $f$ ,

$$ct|f(t)| \leq \frac{2c\|h\|_\infty \mathbb{P}[X \geq t]}{p(t)} \leq \frac{\|h\|_\infty}{3t} \left( 1 + \frac{2}{3ct^2} + \frac{2}{9c^2t^4} \right),$$

making use again of the estimate  $\mathbb{P}[X \geq t] \leq \frac{p(t)}{6ct} \left( 1 + \frac{2}{3ct^2} + \frac{2}{9c^2t^4} \right)$ . Taking  $t_o = \sqrt{\frac{5}{6c}}$  as before and making some trivial simplifying estimates completes the proof of this part.

(c) Differentiating both sides of the Stein equation gives that

$$tf''(t) = 12ctf(t) + (6ct^2 - 7)f'(t) + h'(t). \quad (20)$$

If  $t \leq t_o$ , then  $|12ctf(t)| \leq 5c\|h\|_\infty$  and by the Stein equation,  $|6ctf'(t)| \leq 36c\|f\|_\infty + 12c\|h\|_\infty \leq 192c\|h\|_\infty$ . Also by the Stein equation,

$$f'(t) = 6f(t) \left( ct - \frac{1}{t} \right) + \frac{h(t) - \mathbb{E}h(X)}{t}.$$

The first term can be absorbed into the existing bound, so that

$$|f''(t)| \leq C\|h\|_\infty + \frac{1}{t} \left| h'(t) + \frac{42f(t) - 7[h(t) - \mathbb{E}h(X)]}{t} \right|.$$

(From now on we will not bother to keep track of specific constants and their dependence on  $c$ .) Now,

$$\begin{aligned}
h'(t) - \frac{7[h(t) - \mathbb{E}h(X) - 6f(t)]}{t} \\
&= h'(t) - \frac{42}{t^2 p(t)} \int_0^t \left( [h(t) - \mathbb{E}h(X)] \frac{s^5 p(t)}{t^5} - [h(s) - \mathbb{E}h(X)] p(s) \right) ds \\
&= -\frac{42}{t^2 p(t)} \int_0^t \left( [h(t) - \mathbb{E}h(X)] \frac{s^5 p(t)}{t^5} - [h(s) - \mathbb{E}h(X)] p(s) - \frac{(t-s)s^5 h'(t) p(t)}{t^5} \right) ds \\
&= -\frac{42}{t^2 p(t)} \int_0^t \left( [h(t) - \mathbb{E}h(X)] e^{-3ct^2} - [h(s) - \mathbb{E}h(X)] e^{-3cs^2} - (t-s)h'(t) e^{-3ct^2} \right) \frac{s^5}{z} ds.
\end{aligned}$$

Let  $H(t) := [h(t) - \mathbb{E}h(X)] e^{-3ct^2}$ . Then

$$H'(t) = [h'(t) - 6ct[h(t) - \mathbb{E}h(X)]] e^{-3ct^2},$$

and so the equation above becomes

$$\begin{aligned}
h'(t) - \frac{7[h(t) - \mathbb{E}h(X) - 6f(t)]}{t} \\
&= \frac{42}{t^2 p(t)} \int_0^t \left( H(s) - H(t) - (s-t)H'(t) + 6ct(t-s)[h(t) - \mathbb{E}h(X)] e^{-3ct^2} \right) \frac{s^5}{z} ds.
\end{aligned}$$

It follows that

$$\left| h'(t) - \frac{7[h(t) - \mathbb{E}h(X) - 6f(t)]}{t} \right| \leq \frac{42}{t^2 p(t)} \left[ \left( \sup_{s \in (0,t)} |H''(s)| \right) \left( \frac{t^8}{12z} \right) + \frac{ct^8}{z} [h(t) - \mathbb{E}h(X)] e^{-3ct^2} \right].$$

Now,

$$H''(s) = [h''(s) - 12csh'(s) - 6c(6cs^2 - 1)[h(s) - \mathbb{E}h(X)]] e^{-3cs^2},$$

so

$$\sup_{s \in (0,t)} |H''(s)| \leq \|h''\|_\infty + 12ct_o \|h'\|_\infty + 24c \|h\|_\infty.$$

All together, this gives that for  $t \leq t_o$ ,

$$|f''(t)| \leq C_1 \|h\|_\infty + C_2 \|h'\|_\infty + \|h''\|_\infty,$$

where  $C_1, C_2, C_3$  are constants depending only on  $c$ .

For  $t > t_o$ , it follows from (20) and estimates already carried out that

$$\begin{aligned}
|f''(t)| &\leq 12c \|f\|_\infty + \left( 6ct + \frac{7}{t_o} \right) |f'(t)| + \frac{\|h'\|_\infty}{t_o} \\
&\leq C_4 \|h\|_\infty + C_5 \|h'\|_\infty + ct |f'(t)|.
\end{aligned}$$

By the Stein equation,

$$ctf'(t) = 6cf(t)(ct^2 - 1) + ch(t) - c\mathbb{E}h(X),$$

and

$$|c^2t^2f(t)| \leq \frac{2c^2t\|h\|_\infty\mathbb{P}[X \geq t]}{p(t)} \leq \frac{c\|h\|_\infty}{3} \left(1 + \frac{2}{3ct^2} + \frac{2}{9c^2t^4}\right),$$

and so finally

$$|f''(t)| \leq C_6\|h\|_\infty + C_4\|h'\|_\infty.$$

□

With the boundedness lemma, we can now give the proof of Theorem 12. For convenience, we recall the statement.

**Theorem 12.** *Let  $(W, W')$  be an exchangeable pair of positive random variables. Suppose there exists a  $\sigma$ -field  $\mathcal{F} \supseteq \sigma(W)$  and  $k > 0$  deterministic such that*

$$\mathbb{E}[W' - W | \mathcal{F}] = 3k(1 - cW^2) + E$$

and

$$\mathbb{E}[(W' - W)^2 | \mathcal{F}] = kW + E'.$$

Let  $X$  have density

$$p(t) = \begin{cases} \frac{1}{z}x^5e^{-\frac{ct^2}{2}} & t \geq 0; \\ 0 & t < 0. \end{cases}$$

Then there are constants  $C_1, C_2, C_3$  depending only on  $c$  such that for all  $h \in C^2(\mathbb{R})$ ,

$$\begin{aligned} |\mathbb{E}h(W) - \mathbb{E}h(X)| &\leq \frac{C_1\|h\|_\infty}{k}\mathbb{E}|E| + \left(\frac{C_2(\|h\|_\infty + \|h'\|_\infty)}{k}\right)\mathbb{E}|E'| \\ &\quad + \left(\frac{C_3(\|h\|_\infty + \|h'\|_\infty + \|h''\|_\infty)}{k}\right)\mathbb{E}|W' - W|^3. \end{aligned}$$

*Proof.* Given  $h$ , let  $f$  be the solution to the Stein equation described above. Then by exchangeability and the conditions on  $(W, W')$ ,

$$\begin{aligned} 0 &= \mathbb{E}[(W' - W)(f(W') + f(W))] \\ &= \mathbb{E}[(W' - W)(f(W') - f(W)) + 2(W' - W)f(W)] \\ &= \mathbb{E}[(W' - W)^2f'(W) + E'' + 6k(1 - cW^2)f(W) + 2Ef(W)] \\ &= \mathbb{E}[kWf'(W) + E'f'(W) + E'' + 6k(1 - cW^2)f(W) + 2Ef(W)]. \end{aligned}$$

Then

$$\mathbb{E}[Wf'(W) + 6(1 - cW^2)f(W)] = -\frac{1}{k}\mathbb{E}[E'f'(W) + 2Ef(W) + E''],$$

and

$$|E''| \leq \frac{\|f''\|_\infty}{2}|(W' - W)|^3.$$

The result is thus immediate from Lemma 18.

□

## 7 Acknowledgments

The authors thank Enzo Marinari and Giovanni Gallavotti for illuminating discussions.

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